# ON REGULARIZATION OF LEAST SQUARE PROBLEMS VIA QUADRATIC CONSTRAINTS

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## ABSTRACT

We consider uncertainty reduction in least square problems raised in system identification with unknown state space. We assume existence of some prior information obtained through a finite series of measurements. This data is modeled in the form of a finite collection of quadratic constraints enclosing the state space. A simple closed form expression is derived for the optimal solution featuring geometric insights and intuitions that reveal a two-fold effort in reducing uncertainty: by correcting the observation error and by improving the condition number of the data matrix. To deal with the dual problem of finding the optimal Lagrange multipliers, we introduce an approximate, positive semidefinite program that can be easily solved using the standard numerical techniques.

***Index Terms***— Identification, least squares methods, linear systems, uncertainty, and regularization.

## 1. INTRODUCTION

Least square problems arise in many applications in signal processing and control including linear system identification. The common ingredients in these problems are a domain $\mathcal{X} \subset \mathbb{R}^n$ which is a compact set denoting the *state space*, a range $\mathcal{Y} = \mathbb{R}^m$ denoting the *observation space*, and a linear mapping $A\colon \mathcal{X} \to \mathcal{Y}$ denoting the *data matrix*. In many practical scenarios, the state space $\mathcal{X}$ is either unknown or its description is very difficult. The problem is posed as there is an unknown underlying element $x^* \in \mathcal{X}$, whose image $Ax^* \in \mathcal{Y}$ under the operation of an input data matrix $A$ is available subject to some additive noise in the form $b = Ax^* + v$. The objective is to use the given knowledge on $A$ and $b$ and to find a good estimate for $x^*$. A basic approach is to assume $\mathcal{X} = \mathbb{R}^m$ and solve

$$\inf_{x\in\mathcal{X}} \|Ax - b\|^2 \tag{1}$$

that results to the least square solution

$$x_{\mathrm{LS}} = A^+ b, \tag{2}$$

where $A^+$ denotes the pseudoinverse of $A$. This solution, however, could harbor a high degree of uncertainty, depending on the amount of observation noise in $b$ and a potential rank deficient or ill-conditioned data matrix $A$. More specifically, if we assume $\|Ax^* - b\| \leq \delta$, for some $\delta > 0$, and assuming that $A = \sum_{i=1}^n \sigma_i u_i v_i'$ denotes the singular value decomposition (SVD) of $A$, the uncertainty in any direction $v_i$ of the least square solution would be smaller than or equal to $\frac{\delta}{\sigma_i}$ that could be quite large for small singular values, even for very small $\delta > 0$. A comprehensive error analysis for least square problems can be found in [1], [2].

To reduce the uncertainty, some information on $\mathcal{X}$ or some additional required features needs to be incorporated in the search for solution. This is the essence of many *regularization* techniques like *Tikhonov regularization* and *constrained optimization* [1], [2], [3]. In the latter one, in particular, (1) is modified to

$$\inf_{x\in\mathcal{X}_\eta} \|Ax - b\|^2, \tag{3}$$

for some compact constraint set $\mathcal{X}_\eta$ such that $\mathcal{X} \subseteq \mathcal{X}_\eta$ whose tightness is controlled by some parameter $\eta \geq 0$. The key is how to use the prior knowledge and define a good $\mathcal{X}_\eta$. From an information perspective, i.e., reducing uncertainty, $\mathcal{X}_\eta$ should be tight and comprehensive. From a computational point of view, it should be simple and concise, as membership verification for some sets could be NP-hard. This has been the general theme of much work in the literature including set theoretic estimation [4] and set membership identification [5]. In the tradeoff between these two requirements, a basic geometrical shape that is commonly used often is ellipsoid.

In this paper, we model the prior information in the form of a finite collection of ellipsoids that enclose the unknown state space. While there has been a decent amount of work on recursive numerical solutions for such problems, also known as quadratic programs with quadratic constraints (QPQC) [3], solving these problems through derivation of an analytical formula has not attracted much attention as it requires solving for Lagrange multipliers through a nonlinear program. This, in particular, becomes more challenging as the number of constraining ellipsoids increases. In fact, some existing work that somehow simplifies this problem is through the assumption that there are uncountable constraining ellipsoids in any directions within a bounded variation [6]. This essentially creates a spherical cross section among all ellipsoids and simplifies the problem into a single spherical constraint.

In this paper, we take an analytical approach for the regularization of least square problems with a finite number of ellipsoids. For this purpose, we extend the dimension of the state space by one to deal with a collection of concentric ellipsoids. This helps to provide important geometrical insights and intuitions as well as derivation of a simple, closed form expression for the optimal solution. The obtained solution reveals a two-fold effort in dealing with uncertainty by correcting the observation error and by improving the condition number of the data matrix. The other advantage of this extension is yielding to a dual problem with simple nonlinear expression that with some manipulation is converted into an approximate, positive semidefinite program that can be easily solved. The approximate dual program is quite insightful and intuitive that helps to simplify the problem even more prior to obtaining the numerical solution.

## 2. SETUP AND PROBLEM FORMULATION

Since the states in a physical system have bounded energy, we may assume that $\mathcal{X}$ is a compact, convex space contained in the unit ball. We assume that there is a calibration phase comprising a finite number of steps where at each step the system changes its state and after each change, we can send certain signals into the system and observe the noisy response of the system to these signals. After each step, indexed by $\theta$, we form the input signal into a (Toeplitz) matrix $A_\theta$ and the output signal into a vector $b_\theta$. Hence, at the end of calibration, after a sufficient number of steps, we obtain a finite collection $\{(A_\theta, b_\theta)\}_{\theta\in\Theta}$ of observations. Note that the number of rows in individual $A_\theta$'s could be different as the time duration of each step could be different.

For a sufficiently large $\eta > 0$, we have $\mathcal{X} \subseteq \mathcal{X}_\eta$ where

$$\mathcal{X}_\eta = \{x \in \mathbb{R}^n : \sup_{\theta\in\Theta} \|A_\theta x - b_\theta\| \leq \eta\}. \tag{4}$$

Provided that there are a sufficient number of steps during the calibration phase and $\eta$ is chosen small enough, then the expression in (4) could be a very tight approximation for $\mathcal{X}$. To emphasize that $\mathcal{X}$ is contained in the unit ball, we define an auxiliary matrix $A_{\theta_0} = \eta I_n$ and $b_{\theta_0} = 0$ and add it to the collection, i.e., $\Theta = \Theta \cup \{\theta_0\}$.

Now, the objective is to solve the least square problem (1) subject to (4). A numerical solution can be derived using standard numerical techniques in the context of QPQC, e.g., interior-point methods [3]. However, the approach of this work is an analytical one as discussed in the following.

### 2.1. Extension of the State Space to a Higher Dimension

Associated with each constraint $\|A_\theta x - b_\theta\|$, we form a positive semidefinite matrix $\tilde{A}'_\theta \tilde{A}_\theta$, where $\tilde{A}_\theta = [A_\theta \ \ -b_\theta]$ is an extended matrix formed by concatenation of $-b_\theta$ to $A_\theta$. Let $\tilde{x} = [x, w] \in \mathbb{R}^{n+1}$ where $w$ is a real value. For every $\theta \in \Theta$

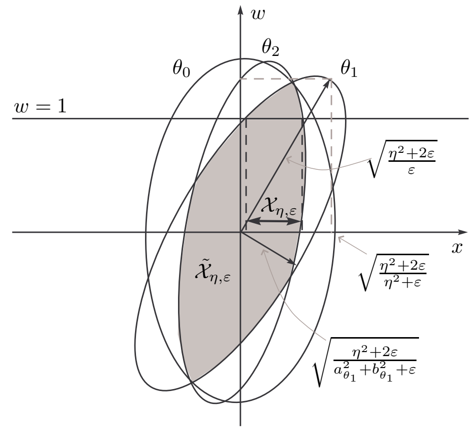



**Fig. 1**: Representation of the subjective constraints in a higher dimension using concentric ellipsoids.

and $\varepsilon \geq 0$, let

$$\tilde{D}_{\theta,\varepsilon} = \tilde{A}'_\theta \tilde{A}_\theta + \varepsilon I, \tag{5}$$

and

$$\tilde{\mathcal{X}}_{\eta,\varepsilon} = \{\tilde{x} \in \mathbb{R}^{n+1} : \sup_{\theta\in\Theta} \tilde{x}' \tilde{D}_{\theta,\varepsilon} \tilde{x} \leq \eta^2 + 2\varepsilon\}.$$

Here, $\varepsilon$ is a *relaxation parameter* added to avoid technical difficulties that rise due to possible rank deficiencies of $\tilde{A}'_\theta \tilde{A}_\theta$. The subset $\tilde{\mathcal{X}}_{\eta,\varepsilon} \subset \mathbb{R}^{n+1}$ is called an *extended enclosing set* associated with $\Theta$, $\eta$, and relaxation parameter $\varepsilon$. Figure 1 illustrates a two dimensional example showing the extended enclosing set at the intersection of a collection of three concentric ellipsoids characterized. Let $\mathcal{X}_{\eta,\varepsilon}$ denote the projection of the intersection of $\tilde{\mathcal{X}}_{\eta,\varepsilon}$ and the hyperplane $w = 1$ onto $\mathbb{R}^n$, as shown in Figure 1. It can be verified that $\mathcal{X} \subseteq \mathcal{X}_{\eta,\varepsilon}$ for all $\varepsilon > 0$, and $\mathcal{X}_{\eta,\varepsilon_1} \subseteq \mathcal{X}_{\eta,\varepsilon_2}$, if $\varepsilon_1 \leq \varepsilon_2$.

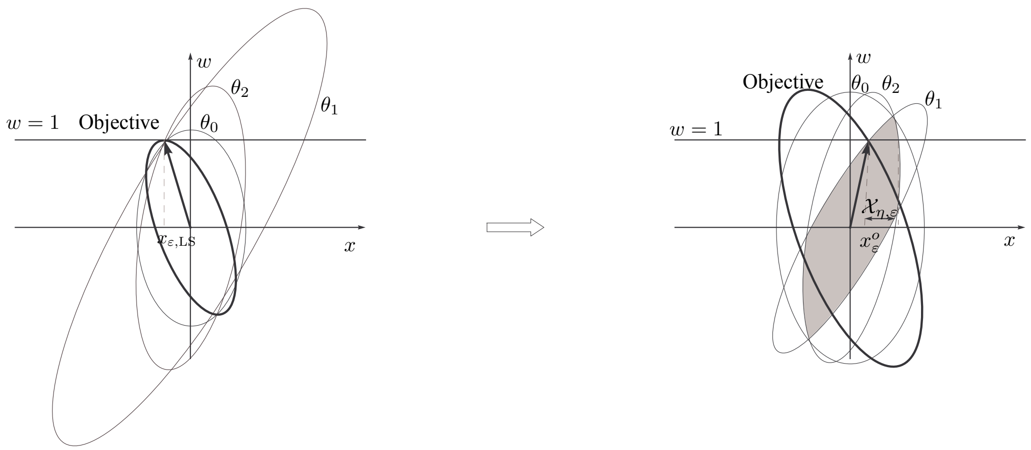
From Figure 1, it appears that the auxiliary restriction indexed by $\theta_0$ is not active at all. In fact, for every given pair $\theta_1$ and $\theta_2$ if $\tilde{A}'_{\theta_1}\tilde{A}_{\theta_1} - \tilde{A}'_{\theta_2}\tilde{A}_{\theta_2}$ is positive semidefinite, then constraint $\theta_2$ is *majorized* by $\theta_1$, i.e.,

$$\forall x : \|A_{\theta_2} x - b_{\theta_2}\| \leq \|A_{\theta_1} x - b_{\theta_1}\|.$$

This is equivalent to say the ellipsoid indexed by $\theta_1$ is contained in $\theta_2$ for all $\varepsilon \geq 0$, and hence the constraint indexed by $\theta_2$ is completely inactive and it can be removed from the set of constraints specified by $\{(A_\theta, b_\theta)\}_\Theta$. This could reduce the number of constraints and simplifies the problem.

## 3. ANALYTICAL EXPRESSION FOR SOLUTION

In this section, we formulate an optimization problem using the extended formulation that was introduced in the previous part. Let $\tilde{A} = [A \ \ -b]$ and $\tilde{C}_\varepsilon = \tilde{A}'\tilde{A} + \varepsilon I$. Let $e_{n+1} \in \mathbb{R}^{n+1}$ denote the unit vector whose first $n$ elements are zero. The




(a) Least square

(b) Regularized

**Fig. 2**: Comparing (a) least square solution and (b) regularized solution along with the contours of the subjective constraints.

optimization problem in the extended setting is

$$\begin{aligned} &\inf_{\tilde{x}} \tilde{x}'\tilde{C}_\varepsilon\tilde{x}, \\ &\text{s.t. } \sup_{\theta\in\Theta} \tilde{x}'\tilde{D}_{\theta,\varepsilon}\tilde{x} \le \eta + 2\varepsilon, \text{ and} \\ &\quad 1 - e'_{n+1}\tilde{x} \le 0. \end{aligned} \tag{6}$$

That is instead of solving the least square problem (1) subject to (4), we solve (6) whose solution is given in the following result that is proved based on the strong duality [3].

**Theorem 3.1.** *The optimal solution of* (6) *is*

$$\tilde{x}^o_\varepsilon = \frac{(\tilde{C}_\varepsilon + \lambda_o\tilde{D}^o_\varepsilon)^{-1}e_{n+1}}{e'_{n+1}(\tilde{C}_\varepsilon + \lambda_o\tilde{D}^o_\varepsilon)^{-1}e_{n+1}} \tag{7}$$

*where $\lambda_o$ and $\tilde{D}^o_\varepsilon$ are the optimal solutions of*

$$\sup_{\lambda\ge 0, \tilde{D}_\varepsilon\in\tilde{\mathscr{D}}_{\Theta,\varepsilon}} \frac{1}{e'_{n+1}(\tilde{C}_\varepsilon + \lambda\tilde{D}_\varepsilon)^{-1}e_{n+1}} - \lambda\eta^2, \tag{8}$$

*and $\tilde{\mathscr{D}}_{\Theta,\varepsilon}$ denotes the convex hull*[1] *of $\{\tilde{D}_{\theta,\varepsilon}\}_{\theta\in\Theta}$.*

In other words, Theorem 3.1 states that there exist a matrix $\tilde{D}^o_\varepsilon$ formed by a ceratin convex combination of the elements of $\{\tilde{D}_{\theta,\varepsilon}\}_\Theta$ and a certain scalar $\lambda_o$ that define (7) as the optimal solution for (6). Expression (7) is a simple analytical expression for the optimal solution that relies on the solution of a nonlinear *dual problem* posed by (8). In Subsection 3.2, we will approximate the dual problem with a linear, positive semidefinite program that can be solved more easily.

The optimal extended solution expressed in (7) defines an optimal solution $x^o_\varepsilon$ through its first $n$ elements. Let

$$\tilde{D}^o_\varepsilon = \begin{bmatrix} D^o_\varepsilon & -d^o \\ -d^{o\prime} & e^o_\varepsilon \end{bmatrix} \tag{9}$$

denote the block decomposition of $\tilde{D}^o_\varepsilon$ where $D^o_\varepsilon$, $d^o$, and $e^o_\varepsilon$ belong to convex hulls of $\{A'_\theta A_\theta\}_\Theta + \varepsilon I$, $\{A'_\theta b_\theta\}_\Theta$, and $\{b'_\theta b_\theta\}_\Theta + \varepsilon$, respectively, with the same optimal convex combination weights. Then

$$x^o_\varepsilon = (A'A + \varepsilon I + \lambda_o D^o_\varepsilon)^{-1}(A'b + \lambda_o d^o) \tag{10}$$

defines a regularized least square solution with relaxation $\varepsilon$. For certain problems, $x^o_\varepsilon$ has a continuous bounded behavior with respect to $\varepsilon$. Thus, in those problems, we would have $x^o = \lim_{\varepsilon\to 0} x^o_\varepsilon$ as non-relaxed, regularized least square solution.

Analyzing (10), it turns out there is a two-fold effort on how the constraints combat with the uncertainty. While the term $\lambda_o D^o_\varepsilon$ that added to $A'A$ aims to increase the singular value, an error correction term, $\lambda_o d^o$, is added to $A'b$ to reduce the observation error.

### 3.1. An example

Consider a one dimensional problem, where we would like to solve $\inf |ax - b|$ for $ab < 0$ subject to $|a_{\theta_i}x - b_{\theta_i}| \le \eta$ for $i = 0, 1, 2$, where $a_{\theta_0} = \eta$, $b_{\theta_0} = 0$, $a_{\theta_1}b_{\theta_1} > 0$, $a_{\theta_2}b_{\theta_2} > 0$. Figure 2(b) depicts the contours of the extended constraining ellipsoids specified by (6) along with a contour of extended objective function. The optimal solution $\tilde{x}^o_\varepsilon$ characterized by Theorem 3.1 is shown by a solid arrow in the intersection of the ellipsoid indexed by $\theta_1$ and the line $w = 1$. The corresponding solution $x^o_\varepsilon$ is shown as projection of $\tilde{x}_o$ on the $x$-axis. Since $\theta_0$ and $\theta_2$ are not active constraints, we have

$$x^o_\varepsilon = \frac{a_{\theta_1}b_{\theta_1} - \sqrt{(a^2_{\theta_1} + \varepsilon)(\eta^2 + \varepsilon) - b^2_{\theta_1}\varepsilon}}{a^2_{\theta_1} + \varepsilon}. \tag{11}$$

By continuity with respect to $\varepsilon$, we obtain

$$x^o = \lim_{\varepsilon\to 0} x^o_\varepsilon = \frac{b_{\theta_1} - \eta}{a_{\theta_1}}. \tag{12}$$

In contrast, in Figure 2(a), a modified least square scenario is depicted where (6) is solved without considering the ellipsoidal constraints. In this case, we obtain a least square

[1] The convex hull of a set of elements is a set containing all possible convex combinations of its elements.

solution with $\varepsilon$ relaxation $x_{\varepsilon,\mathrm{LS}} = \frac{ab}{a^2+\varepsilon}$, where by continuity $x_{\mathrm{LS}} = \lim_\varepsilon x_{\varepsilon,\mathrm{LS}} = \frac{b}{a}$. One can compare the contours corresponding to constraint $\theta_1$ in Figure 2 and notice that there is quite a large amount of error shown in constraint $\theta_1$ for $x_{\varepsilon,\mathrm{LS}}$. This indicates that for the choice of least square solution the maximum amount of error occurs for the ellipsoidal constraint that has its maximum singular vector aligned with the minimum singular vector of the objective function. In other words, in the optimal solution, we can expect to have more contribution from those constraints, $\tilde{A}'_\theta A_\theta$, whose larger singular values are aligned with smaller singular values of the objective function $\tilde{A}'A$.

### 3.2. Approximating the Dual Problem

With some straightforward manipulation, we rephrase the dual problem (8) as

$$\sup\ t\ \text{ s. t.}$$
$$e'_{n+1}\Big[I - (\lambda\eta^2 + t)(\tilde{C}_\varepsilon + \lambda\tilde{D}_\varepsilon)^{-1}\Big]e_{n+1} \geq 0, \quad (13)$$

where $t$ is a real valued slack variable. This problem, however, is still a non-linear optimization problem. Although, a numerical solution of (13) would determine $\tilde{D}^o_\varepsilon$ and $\lambda_o$, to provide intuitive arguments and simplify the problem, we replace (13) with an optimization with stricter conditions as

$$\sup\ t\ \text{ s. t. }\ \tilde{C}_\varepsilon + \lambda\tilde{D}_\varepsilon - (\lambda\eta^2 + t)I \succcurlyeq 0. \qquad (14)$$

The problem posed in (14) is a linear, positive semidefinite program (SDP) that can be easily solved using numerical techniques known for these programs [3]. Thus, we focus on implications and insights that can be obtained from (14). For this purpose, we expand (14) by substituting for $\tilde{D}_\varepsilon$ and $\tilde{C}_\varepsilon$ using a set of nonnegative real values $\{\lambda_i\}_{i=1}^{|\Theta|}$ ($\lambda = \sum \lambda_i$) to obtain

$$\sum_i \lambda_i\Big(\tilde{A}'_{\theta_i}\tilde{A}_{\theta_i} - (\eta^2 - \varepsilon)I\Big) \succcurlyeq (t - \varepsilon)I - \tilde{A}'\tilde{A}. \qquad (15)$$

From (15), it turns out that for certain choices of $\eta$ and $\varepsilon$, in particular for sufficiently small $\eta$, there could exist some $\theta_i$ such that $\tilde{A}'_{\theta_i}\tilde{A}_{\theta_i} \succcurlyeq (\eta^2 - \varepsilon)I$. Hence, the corresponding $\lambda_i$ could grow unbounded implying that $t$ would be infinite. In this case, an optimal solution for (14) would be trivial. One can simply pick $\tilde{D}^o_\varepsilon = \tilde{A}'_{\theta_i}\tilde{A}_{\theta_i} + \varepsilon I$ and $\lambda_o$ a very large value obtaining

$$x^o_\varepsilon \approx (\tilde{D}^o_\varepsilon)^{-1}d^o.$$

This basically means that if (4) is inappropriately very tight, then the solution would suffer from a large approximation error. In the other extreme, if the choice of $\eta$ and $\varepsilon$ are such that $(\eta^2 - \varepsilon)I$ completely dominates every $\tilde{D}_\varepsilon$, then $\lambda$ needs to be very small. As a result, asymptotically as $\eta \to \infty$, the constraining set (4) becomes very loose and $x^o \to x_{\mathrm{LS}}$.

Unlike these extreme cases, for appropriate choices of $\eta$, the solution of (14) is not trivial and one needs to solve the linear, positive semidefinite program posed in (14) to find $t$ and $\lambda_i$'s. However, it can be intuitively argued that the weighting selection of $\theta_i$'s should emphasize more on those $\tilde{A}'_{\theta_i}\tilde{A}_{\theta_i}$ that have their larger singular values aligned with smaller singular values of $\tilde{A}'\tilde{A}$, which is in complete agreement of our observation and inference from Figure 2.

Although, the complexity of this problem could potentially grow by $|\Theta|$, the problem can be simplified by the notion of majorization mentioned in Section 2.1 as well as the Caratheodory's Theorem [7] stating that any point in $\tilde{\mathscr{D}}_{\Theta,\varepsilon}$ can be written as a convex combination of a maximum

$$\min(\lceil\frac{(m+1)n}{2}\rceil + 1, |\Theta|)$$

number of linearly independent vertices of $\{\tilde{D}_{\theta,\varepsilon}\}_\Theta$. That is there exists an optimal setting of $\lambda_i$'s that has at most the minimum of $|\Theta|$ and $\lceil\frac{(m+1)n}{2}\rceil + 1$ nonzero elements.

## 4. CONCLUSION

In this work, we considered the problem of regularizing least square optimization using prior information that is modeled as a finite number of quadratic constraints. The problem was extended to a higher dimensional space that led to the derivation of a simple, closed form expression for the regularized solution. The solution is expressed in terms of Lagrange multipliers whose solutions are obtained through a nonlinear dual problem. To simplify the search for Lagrange multipliers, the dual problem is approximated with a linear, positive semidefinite program that can be easily solvable through standard techniques. The approximation problem provides important insights that are in full agreement with prior observations and intuitions. Further insights and rigorous accuracy assessment of the approximation problem remain to future work.

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