Technical Note: Formulations for Constrained Least Squares Optimization

This note explores different mathematical formulations for solving the constrained least squares optimization problem:

$$\min_x |Cx - b|_2 \quad \text{subject to} \quad Ax = d, \quad Gx \geq f$$

where $C \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$, $A \in \mathbb{R}^{p \times n}$, $d \in \mathbb{R}^p$, $G \in \mathbb{R}^{q \times n}$, $f \in \mathbb{R}^q$, and $m \gg n$.

1. Direct Quadratic Programming Approach (direct)

The 2-norm can be squared to obtain a standard quadratic programming formulation:

$$\min_x |Cx - b|_2 = \min_x |Cx - b|_2^2 = \min_x \, (Cx - b)^T (Cx - b)$$

Expanding gives $(Cx - b)^T (Cx - b) = x^T C^T C x - 2 b^T C x + b^T b$.

The constant term does not affect the minimization, so we can drop it. We get

$$\min_x \, x^T C^T C x - 2 b^T C x \quad \text{subject to} \quad Ax = d, \quad Gx \geq f.$$

This can be written in standard form as:

$$\min_x \, \tfrac{1}{2} x^T P x + q^T x \quad \text{subject to} \quad Ax = d, \quad Gx \geq f$$

where $P = 2 C^T C$ and $q = -2 C^T b$.

Note on numerical issues: While dropping the constant term $b^T b$ is mathematically valid, it can lead to numerical issues when $|b|$ is large. The objective function value is offset by a large constant, which may cause convergence criteria to behave poorly.

KKT System Dimensionality: The KKT system for this approach involves:
- n variables from the original problem
- p dual variables for equality constraints
- Up to q dual variables for inequality constraints.

The resulting KKT matrix has dimensions $(n + p + q) \times (n + p + q)$.

2. Variable Splitting Method (splitting)

We introduce auxiliary variables $r \in \mathbb{R}^m$ where $r = Cx - b$, and get

$$\min_{x,r} |r|_2^2 \quad \text{subject to} \quad r = Cx - b, \quad Ax = d, \quad Gx \geq f.$$

This formulation uses additional variables to avoid the numerical issues of the previous approach.

KKT System Dimensionality: The KKT system for this approach involves:
- $n + m$ primal variables (n from x and m from r)
- m dual variables for the constraint $r = Cx - b$
- p dual variables for equality constraints $Ax = d$
- Up to q dual variables for inequality constraints $Gx \geq f$

The resulting KKT matrix has dimensions $(n + 2m + p + q) \times (n + 2m + p + q)$.

3. Variable splitting with Dimension Reduction via QR (reduced-splitting-qr)

In this approach, we use an economic QR decomposition of C to reduce the dimensionality of the problem:

$$C = QR$$

where $Q \in \mathbb{R}^{m \times n}$ has orthonormal columns and $R \in \mathbb{R}^{n \times n}$ is upper triangular.

We introduce new variables $\hat{r} \in \mathbb{R}^n$ defined as:

$\hat{r} = Rx - Q^T b$

Our problem becomes:

$\min_{x,\hat{r}} |\hat{r}|_2 \quad \text{subject to} \quad \hat{r} = Rx - Q^T b, \quad Ax = d, \quad Gx \geq f.$

Proof of Equivalence
We need to show that minimizing $|\hat{r}|_2$ with the constraint $\hat{r} = Rx - Q^T b$ leads to the same minimizer as the original problem $\min_x |Cx - b|_2$.

Starting from the original objective $|Cx - b|_2 = |QRx - b|_2$.

Since Q has orthonormal columns, we can decompose b into a component in the column space of Q and a component orthogonal to it:

$b = QQ^T b + (I - QQ^T) b$

This gives

$|QRx - b|_2 = |QRx - QQ^T b - (b - QQ^T b)|_2.$

Since $QRx - QQ^T b$ is in the column space of Q and $b - QQ^T b$ is orthogonal to it we get $|QRx - b|_2^2 = |QRx - QQ^T b|_2^2 + |b - QQ^T b|_2^2$.

The second term $|b - QQ^T b|_2^2$ is independent of x, so it doesn't affect the minimizer. But the first term is $|QRx - QQ^T b|_2^2 = |Q\hat{r}|_2^2 = \hat{r}^T Q^T Q \hat{r} = |\hat{r}|_2$, because the columns of Q are orthonormal.

KKT System Dimensionality: The KKT system for this approach involves:
- $n + n$ primal variables (n from x and n from $\hat{r}$)
- n dual variables for the constraint $\hat{r} = Rx - Q^T b$
- p dual variables for equality constraints $Ax = d$
- Up to q dual variables for inequality constraints $Gx \geq f$

The resulting KKT matrix has dimensions $(3n + p + q) \times (3n + p + q)$.

4. Second-Order Cone Programming (socp)
We can reformulate the original problem as a second-order cone program using the epigraph form:

$\min_{x,t} t \quad \text{subject to} \quad |Cx - b|_2 \leq t, \quad Ax = d, \quad Gx \geq f.$

This is equivalent to:

$\min_{x,t} t \quad \text{subject to} \quad (Cx - b, t) \in \mathcal{Q}^{m+1}, \quad Ax = d, \quad Gx \geq f$

where $\mathcal{Q}^{m+1}$ is the second-order cone in $\mathbb{R}^{\{m+1\}}$.

This formulation allows the use of SOCP solvers.

KKT System Dimensionality: The KKT system for the SOCP formulation involves:
- $n + 1$ primal variables (n from x and 1 from t)
- $m + 1$ dual variables for the second-order cone constraint
- p dual variables for equality constraints
- Up to q dual variables for inequality constraints

The resulting KKT matrix has dimensions $(n + m + p + q + 2) \times (n + m + p + q + 2)$.