11. Constrained least squares

- least norm problem
- least squares with equality constraints
- linear quadratic control
Least norm problem

minimize $\|x\|^2$
subject to $Cx = d$

- $C$ is a $p \times n$ matrix, $d$ is a $p$-vector
- in most applications $p < n$ and the equation $Cx = d$ is underdetermined
- the goal is to find the solution of the equation $Cx = d$ with the smallest norm

we will assume that $C$ has linearly independent rows

- the equation $Cx = d$ has at least one solution for every $d$
- $C$ is wide or square ($p \leq n$)
- if $p < n$ there are infinitely many solutions
• unit mass, with zero initial position and velocity

• piecewise-constant force $F(t) = x_j$ for $t \in [j - 1, j)$ for $j = 1, \ldots, 10$

• position and velocity at $t = 10$ are given by $y = Cx$ where

$$C = \begin{bmatrix} 19/2 & 17/2 & 15/2 & \cdots & 1/2 \\ 1 & 1 & 1 & \cdots & 1 \end{bmatrix}$$
Example

forces that move mass over a unit distance with zero final velocity satisfy

\[
\begin{bmatrix}
19/2 & 17/2 & 15/2 & \cdots & 1/2 \\
1 & 1 & 1 & \cdots & 1
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2 \\
x_3 \\
\vdots \\
x_{10}
\end{bmatrix} =
\begin{bmatrix}
1 \\
0
\end{bmatrix}
\]

some interesting solutions:

- solutions with only two nonzero elements:

  \[x = (1, -1, 0, \ldots, 0), \quad x = (0, 1, -1, \ldots, 0), \quad \ldots\]

- least norm solution: minimizes

  \[
  \int_0^{10} F(t)^2 dt = x_1^2 + x_2^2 + \cdots + x_{10}^2
  \]
Example

\[ x = (1, -1, 0, \ldots, 0) \]

Least norm solution
Least distance solution

as a variation, we can minimize the distance to a given point \( a \neq 0 \):

\[
\begin{align*}
\text{minimize} & \quad \|x - a\|^2 \\
\text{subject to} & \quad Cx = d 
\end{align*}
\]

- reduces to least norm problem by a change of variables \( y = x - a \)

\[
\begin{align*}
\text{minimize} & \quad \|y\|^2 \\
\text{subject to} & \quad Cy = d - Ca 
\end{align*}
\]

- from least norm solution \( y \), we obtain solution \( x = y + a \) of first problem
Solution of least norm problem

if $C$ has linearly independent rows (is right-invertible), then

$$\hat{x} = C^T(CC^T)^{-1}d$$

$$= C^\dagger d$$

is the unique solution of the least norm problem

$$\minimize \|x\|^2$$

subject to $Cx = d$

• in other words if $Cx = d$ and $x \neq \hat{x}$, then $\|x\| > \|\hat{x}\|$

• recall from page 4.26 that

$$C^T(CC^T)^{-1} = C^\dagger$$

is the pseudo-inverse of a right-invertible matrix $C$
Proof

1. we first verify that \( \hat{x} \) satisfies the equation:

\[
C\hat{x} = CC^T(CC^T)^{-1}d = d
\]

2. next we show that \( \|x\| > \|\hat{x}\| \) if \( Cx = d \) and \( x \neq \hat{x} \)

\[
\|x\|^2 = \|\hat{x} + x - \hat{x}\|^2 \\
= \|\hat{x}\|^2 + 2\hat{x}^T(x - \hat{x}) + \|x - \hat{x}\|^2 \\
= \|\hat{x}\|^2 + \|x - \hat{x}\|^2 \\
\geq \|\hat{x}\|^2
\]

with equality only if \( x = \hat{x} \)

on line 3 we use \( Cx = C\hat{x} = d \) in

\[
\hat{x}^T(x - \hat{x}) = d^T(CC^T)^{-1}C(x - \hat{x}) = 0
\]
QR factorization method

use the QR factorization \( C^T = QR \) of the matrix \( C^T \):

\[
\hat{x} = C^T(CC^T)^{-1}d \\
= QR(R^TQ^TQR)^{-1}d \\
= QR(R^TR)^{-1}d \\
= QR^{-T}d
\]

Algorithm

1. compute QR factorization \( C^T = QR \) (2\( p^2n \) flops)
2. solve \( R^Tz = d \) by forward substitution (\( p^2 \) flops)
3. matrix-vector product \( \hat{x} = Qz \) (2\( pn \) flops)

complexity: 2\( p^2n \) flops
Example

\[ C = \begin{bmatrix} 1 & -1 & 1 & 1 \\ 1 & 0 & 1/2 & 1/2 \end{bmatrix}, \quad d = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \]

- QR factorization \( C^T = QR \)

\[
\begin{bmatrix} 1 & 1 \\ -1 & 0 \\ 1 & 1/2 \\ 1 & 1/2 \end{bmatrix} = \begin{bmatrix} 1/2 & 1/\sqrt{2} \\ -1/2 & 1/\sqrt{2} \\ 1/2 & 0 \\ 1/2 & 0 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix}
\]

- solve \( R^T z = b \)

\[
\begin{bmatrix} 2 & 0 \\ 1 & 1/\sqrt{2} \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}
\]

\( z_1 = 0, \ z_2 = \sqrt{2} \)

- evaluate \( \hat{x} = Qz = (1, 1, 0, 0) \)
Outline

• least norm problem

• least squares with equality constraints

• linear quadratic control
Constrained least squares

minimize $\|Ax - b\|^2$
subject to $Cx = d$

- $A$ is an $m \times n$ matrix, $C$ is a $p \times n$ matrix, $b$ is an $m$-vector, $d$ is a $p$-vector
- in most applications $p < n$, so equations are underdetermined
- the goal is to find the solution of $Cx = d$ with smallest value of $\|Ax - b\|^2$
- we make no assumptions about the shape of $A$

Special cases

- least squares problem is a special case with $p = 0$ (no constraints)
- least norm problem is a special case with $A = I$ and $b = 0$
Piecewise-polynomial fitting

- fit two polynomials $f(x)$, $g(x)$ to points $(x_1, y_1), \ldots, (x_N, y_N)$

$$f(x_i) \approx y_i \quad \text{for points } x_i \leq a, \quad g(x_i) \approx y_i \quad \text{for points } x_i > a$$

- make values and derivatives continuous at point $a$: $f(a) = g(a)$, $f'(a) = g'(a)$

![Diagram showing two polynomials of degree 4](image-url)
Constrained least squares formulation

- assume points are numbered so that $x_1, \ldots, x_M \leq a$ and $x_{M+1}, \ldots, x_N > a$:

  \[
  \begin{align*}
  \text{minimize} & \quad \sum_{i=1}^{M} (f(x_i) - y_i)^2 + \sum_{i=M+1}^{N} (g(x_i) - y_i)^2 \\
  \text{subject to} & \quad f(a) = g(a), \quad f'(a) = g(a)
  \end{align*}
  \]

- for polynomials $f(x) = \theta_1 + \cdots + \theta_d x^{d-1}$ and $g(x) = \theta_{d+1} + \cdots + \theta_{2d} x^{d-1}$

\[
A = \begin{bmatrix}
1 & x_1 & \cdots & x_1^{d-1} & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
1 & x_M & \cdots & x_M^{d-1} & 0 & 0 & \cdots & 0 \\
0 & 0 & \cdots & 0 & 1 & x_{M+1} & \cdots & x_{M+1}^{d-1} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & 0 & 1 & x_N & \cdots & x_N^{d-1}
\end{bmatrix}, \quad b = \begin{bmatrix}
y_1 \\
y_M \\
y_{M+1} \\
y_N
\end{bmatrix}
\]

\[
C = \begin{bmatrix}
1 & a & \cdots & a^{d-1} & -1 & -a & \cdots & -a^{d-1} \\
0 & 1 & \cdots & (d-1)a^{d-2} & 0 & -1 & \cdots & -(d-1)a^{d-2}
\end{bmatrix}, \quad d = \begin{bmatrix}
0 \\
0
\end{bmatrix}
\]
Assumptions

minimize $\|Ax - b\|^2$
subject to $Cx = d$

we will make two assumptions:

1. the stacked $(m + p) \times n$ matrix

$$
\begin{bmatrix}
A \\
C
\end{bmatrix}
$$

has linearly independent columns (is left-invertible)

2. $C$ has linearly independent rows (is right-invertible)

• note that assumption 1 is a weaker condition than left invertibility of $A$
• assumptions imply that $p \leq n \leq m + p$
Optimality conditions

\( \hat{x} \) solves the constrained LS problem if and only if there exists a \( z \) such that

\[
\begin{bmatrix}
AT A & CT \\
C & 0
\end{bmatrix}
\begin{bmatrix}
\hat{x} \\
z
\end{bmatrix}
= \begin{bmatrix}
AT b \\
d
\end{bmatrix}
\]

(proof on next page)

- this is a set of \( n + p \) linear equations in \( n + p \) variables
- we’ll see that the matrix on the left-hand side is nonsingular
- equations are also known as Karush–Kuhn–Tucker (KKT) equations

Special cases

- least squares: when \( p = 0 \), reduces to normal equations \( AT A\hat{x} = AT b \)
- least norm: when \( A = I, \ b = 0 \), reduces to \( C\hat{x} = d \) and \( \hat{x} + C^T z = 0 \)
Proof

suppose \( x \) satisfies \( Cx = d \), and \((\hat{x}, z)\) satisfies the equation on page 11.15

\[
\|Ax - b\|^2 = \|A(x - \hat{x}) + A\hat{x} - b\|^2
\]

\[
= \|A(x - \hat{x})\|^2 + \|A\hat{x} - b\|^2 + 2(x - \hat{x})^T A^T (A\hat{x} - b)
\]

\[
= \|A(x - \hat{x})\|^2 + \|A\hat{x} - b\|^2 - 2(x - \hat{x})^T C^T z
\]

\[
= \|A(x - \hat{x})\|^2 + \|A\hat{x} - b\|^2
\]

\[
\geq \|A\hat{x} - b\|^2
\]

- on line 3 we use \( A^T A\hat{x} + C^T z = A^T b \); on line 4, \( Cx = C\hat{x} = d \)
- inequality shows that \( \hat{x} \) is optimal
- \( \hat{x} \) is the unique optimum because equality holds only if

\[
A(x - \hat{x}) = 0, \quad C(x - \hat{x}) = 0 \implies x = \hat{x}
\]

by the first assumption on page 11.14
Nonsingularity

if the two assumptions hold, then the matrix

\[
\begin{bmatrix}
A^T A & C^T \\
C & 0
\end{bmatrix}
\]

is nonsingular

Proof.

\[
\begin{bmatrix}
A^T A & C^T \\
C & 0
\end{bmatrix}
\begin{bmatrix}
x \\
z
\end{bmatrix} = 0 \implies x^T (A^T A x + C^T z) = 0, \quad C x = 0
\]

\[
\implies \|A x\|^2 = 0, \quad C x = 0
\]

\[
\implies A x = 0, \quad C x = 0
\]

\[
\implies x = 0 \quad \text{by assumption 1}
\]

if \( x = 0 \), we have \( C^T z = -A^T A x = 0 \); hence also \( z = 0 \) by assumption 2
Nonsingularity

if the assumptions do not hold, then the matrix

\[
\begin{bmatrix}
A^T A & C^T \\
C & 0
\end{bmatrix}
\]

is singular

• if assumption 1 does not hold, there exists \( x \neq 0 \) with \( Ax = 0, Cx = 0 \); then

\[
\begin{bmatrix}
A^T A & C^T \\
C & 0
\end{bmatrix} \begin{bmatrix}
x \\
0
\end{bmatrix} = 0
\]

• if assumption 2 does not hold there exists a \( z \neq 0 \) with \( C^T z = 0 \); then

\[
\begin{bmatrix}
A^T A & C^T \\
C & 0
\end{bmatrix} \begin{bmatrix}
0 \\
z
\end{bmatrix} = 0
\]

in both cases, this shows that the matrix is singular
Solution by LU factorization

\[
\begin{bmatrix}
A^T A & C^T \\
C & 0
\end{bmatrix}
\begin{bmatrix}
x \\
z
\end{bmatrix} =
\begin{bmatrix}
A^T b \\
d
\end{bmatrix}
\]

Algorithm

1. compute \( H = A^T A \) (\( mn^2 \) flops)
2. compute \( c = A^T b \) (\( 2mn \) flops)
3. solve the linear equation

\[
\begin{bmatrix}
H & C^T \\
C & 0
\end{bmatrix}
\begin{bmatrix}
x \\
z
\end{bmatrix} =
\begin{bmatrix}
c \\
d
\end{bmatrix}
\]

by the LU factorization (\( (2/3)(p + n)^3 \) flops)

complexity: \( mn^2 + (2/3)(p + n)^3 \) flops
Solution by QR factorization

we derive one of several possible methods based on the QR factorization

\[
\begin{bmatrix}
A^T A & C^T \\
C & 0
\end{bmatrix}
\begin{bmatrix}
\hat{x} \\
z
\end{bmatrix}
= 
\begin{bmatrix}
A^T b \\
d
\end{bmatrix}
\]

• if we make a change of variables \( w = z - d \), the equation becomes

\[
\begin{bmatrix}
A^T A + C^T C & C^T \\
C & 0
\end{bmatrix}
\begin{bmatrix}
\hat{x} \\
w
\end{bmatrix}
= 
\begin{bmatrix}
A^T b \\
d
\end{bmatrix}
\]

• assumption 1 guarantees that \( A^T A + C^T C \) is nonsingular (see page 4.22)

• assumption 1 guarantees that the following QR factorization exists:

\[
\begin{bmatrix}
A \\
C
\end{bmatrix}
= QR = 
\begin{bmatrix}
Q_1 \\
Q_2
\end{bmatrix}
\]

Constrained least squares

11.20
Solution by QR factorization

substituting the QR factorization gives the equation

\[
\begin{bmatrix}
R^T R & R^T Q_2^T \\
Q_2 R & 0 \\
\end{bmatrix}
\begin{bmatrix}
\hat{x} \\
w \\
\end{bmatrix} =
\begin{bmatrix}
R^T Q_1^T b \\
d \\
\end{bmatrix}
\]

• multiply first equation with \(R^{-T}\) and make change of variables \(y = R\hat{x}\):

\[
\begin{bmatrix}
I & Q_2^T \\
Q_2 & 0 \\
\end{bmatrix}
\begin{bmatrix}
y \\
w \\
\end{bmatrix} =
\begin{bmatrix}
Q_1^T b \\
d \\
\end{bmatrix}
\]

• next we note that the matrix \(Q_2 = CR^{-1}\) has linearly independent rows:

\[
Q_2^T u = R^{-T} C^T u = 0 \implies C^T u = 0 \implies u = 0
\]

because \(C\) has linearly independent rows (assumption 2)
Solution by QR factorization

we use the QR factorization of $Q_2^T$ to solve

$$
\begin{bmatrix}
I & Q_2^T \\
Q_2 & 0
\end{bmatrix}
\begin{bmatrix}
y \\
w
\end{bmatrix}
=
\begin{bmatrix}
Q_1^T b \\
d
\end{bmatrix}
$$

• from the 1st block row, $y = Q_1^T b - Q_2^T w$; substitute this in the 2nd row:

$$Q_2 Q_2^T w = Q_2 Q_1^T b - d$$

• we solve this equation for $w$ using the QR factorization $Q_2^T = \tilde{Q} \tilde{R}$:

$$\tilde{R}^T \tilde{R} w = \tilde{R}^T \tilde{Q}^T Q_1^T b - d$$

which can be simplified to

$$\tilde{R} w = \tilde{Q}^T Q_1^T b - \tilde{R}^{-T} d$$
Summary of QR factorization method

\[
\begin{bmatrix}
A^T A + C^T C & C^T \\
C & 0
\end{bmatrix}
\begin{bmatrix}
\hat{x} \\
w
\end{bmatrix}
=
\begin{bmatrix}
A^T b \\
d
\end{bmatrix}
\]

Algorithm

1. compute the two QR factorizations

\[
\begin{bmatrix}
A \\
C
\end{bmatrix}
=
\begin{bmatrix}
Q_1 \\
Q_2
\end{bmatrix} R, \quad Q_2^T = \tilde{Q}\tilde{R}
\]

2. solve \(\tilde{R}^T u = d\) by forward substitution and compute \(c = \tilde{Q}^T Q_1^T b - u\)

3. solve \(\tilde{R} w = c\) by back substitution and compute \(y = Q_1^T b - Q_2^T w\)

4. compute \(R\hat{x} = y\) by back substitution

complexity: \(2(p + m)n^2 + 2np^2\) flops for the QR factorizations
Comparison of the two methods

**Complexity:** roughly the same

- **LU factorization**
  \[ mn^2 + \frac{2}{3}(p + n)^3 \leq mn^2 + \frac{16}{3}n^3 \text{ flops} \]

- **QR factorization**
  \[ 2(p + m)n^2 + 2np^2 \leq 2mn^2 + 4n^3 \text{ flops} \]

upper bounds follow from \( p \leq n \) (assumption 2)

**Stability:** 2nd method avoids calculation of Gram matrix \( A^T A \)
Outline

• least norm problem

• least squares with equality constraints

• linear quadratic control
Linear quadratic control

Linear dynamical system

\[ x_{t+1} = A_t x_t + B_t u_t, \quad y_t = C_t x_t, \quad t = 1, 2, \ldots \]

- \( n \)-vector \( x_t \) is system state at time \( t \)
- \( m \)-vector \( u_t \) is system input
- \( p \)-vector \( y_t \) is system output
- \( x_t, u_t, y_t \) often represent deviations from a standard operating condition

Objective: choose inputs \( u_1, \ldots, u_{T-1} \) that minimizes \( J_{\text{output}} + \rho J_{\text{input}} \) with

\[ J_{\text{output}} = \| y_1 \|^2 + \cdots + \| y_T \|^2, \quad J_{\text{input}} = \| u_1 \|^2 + \cdots + \| u_{T-1} \|^2 \]

State constraints: initial state and (possibly) the final state are specified

\[ x_1 = x^{\text{init}}, \quad x_T = x^{\text{des}} \]
Linear quadratic control problem

minimize \[ \|C_1 x_1\|^2 + \cdots + \|C_T x_T\|^2 + \rho(\|u_1\|^2 + \cdots + \|u_{T-1}\|^2) \]
subject to \[ x_{t+1} = A_t x_t + B_t u_t, \quad t = 1, \ldots, T - 1 \]
\[ x_1 = x^{\text{init}}, \quad x_T = x^{\text{des}} \]

variables: \( x_1, \ldots, x_T, u_1, \ldots, u_{T-1} \)

Constrained least squares formulation

minimize \[ \|\tilde{A} z - \tilde{b}\|^2 \]
subject to \[ \tilde{C} z = \tilde{d} \]

variables: the \((nT + m(T - 1))\)-vector

\[ z = (x_1, \ldots, x_T, u_1, \ldots, u_{T-1}) \]
Linear quadratic control problem

Objective function: $\| \tilde{A}z - \tilde{b} \|^2$ with

$$
\tilde{A} = \begin{bmatrix}
    C_1 & \cdots & 0 & 0 & \cdots & 0 \\
    \vdots & \ddots & \vdots & 0 & \ddots & \vdots \\
    0 & \cdots & C_T & 0 & \cdots & 0 \\
    \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
    0 & \cdots & 0 & 0 & \cdots & \sqrt{\rho}I \\
\end{bmatrix}, \quad \tilde{b} = 0
$$

Constraints: $\tilde{C}z = \tilde{d}$ with

$$
\tilde{C} = \begin{bmatrix}
    A_1 & -I & 0 & \cdots & 0 & 0 & B_1 & 0 & \cdots & 0 \\
    0 & A_2 & -I & \cdots & 0 & 0 & 0 & B_2 & \cdots & 0 \\
    \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\
    0 & 0 & 0 & \cdots & A_{T-1} & -I & 0 & 0 & \cdots & B_{T-1} \\
    I & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\
    0 & 0 & 0 & \cdots & 0 & I & 0 & 0 & \cdots & 0 \\
\end{bmatrix}, \quad \tilde{d} = \begin{bmatrix}
    0 \\
    0 \\
    \vdots \\
    0 \\
    x^{\text{init}} \\
    x^{\text{des}} \\
\end{bmatrix}
$$
Example

- a system with three states, one input, one output
- system is time-invariant (matrices $A_t = A$, $B_t = B$, and $C_t = C$ are constant)
- figure shows “open-loop” output $CA^{t-1}x^{\text{init}}$

- we minimize $J_{\text{output}} + \rho J_{\text{input}}$ with final state constraint $x^{\text{des}} = 0$ at $T = 100$
Optimal trade-off curve

\[ \rho = 0.05 \]
\[ \rho = 0.2 \]
\[ \rho = 1 \]

\( J_{\text{in}} \)
\( J_{\text{out}} \)

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Three solutions on the trade-off curve

\[ \rho = 0.05 \]

\[ \rho = 0.2 \]

\[ \rho = 1 \]
Linear state feedback control

Linear state feedback

- linear state feedback control uses the input

\[ u_t = K x_t, \quad t = 1, 2, \ldots \]

- \( K \) is the state feedback gain matrix
- widely used, especially when \( x_t \) should converge to zero, \( T \) is not specified

One possible choice for \( K \)

- solve the linear quadratic control problem with \( x^{\text{des}} = 0 \)
- solution \( u_t \) is a linear function of \( x^{\text{init}} \), hence \( u_1 \) can be written as \( u_1 = K x^{\text{init}} \)
- columns of \( K \) can be found by computing \( u_1 \) for \( x^{\text{init}} = e_1, \ldots, e_n \)
- use this \( K \) as state feedback gain matrix
• system matrices of previous example

• blue curve uses optimal linear quadratic control for $T = 100$

• red curve uses simple linear state feedback $u_t = Kx_t$