11. Constrained least squares

- least norm problem

- least squares with equality constraints

- linear quadratic control

Least norm problem

$$\begin{array}{ll} \text{minimize} & \|x\|^2 \\ \text{subject to} & Cx = d \end{array}$$

- 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

Example

example of page 1.23
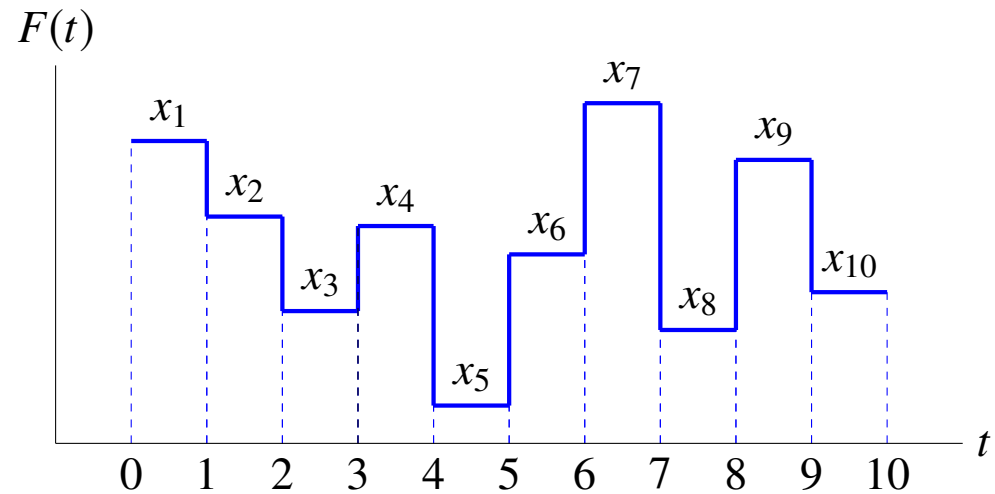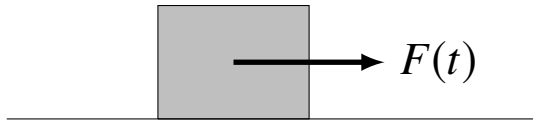
- unit mass, with zero initial position and velocity

- 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

$$\begin{bmatrix} 19/2 & 17/2 & 15/2 & \cdots & 1/2 \\ 1 & 1 & 1 & \cdots & 1 \end{bmatrix} x = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

some interesting solutions:

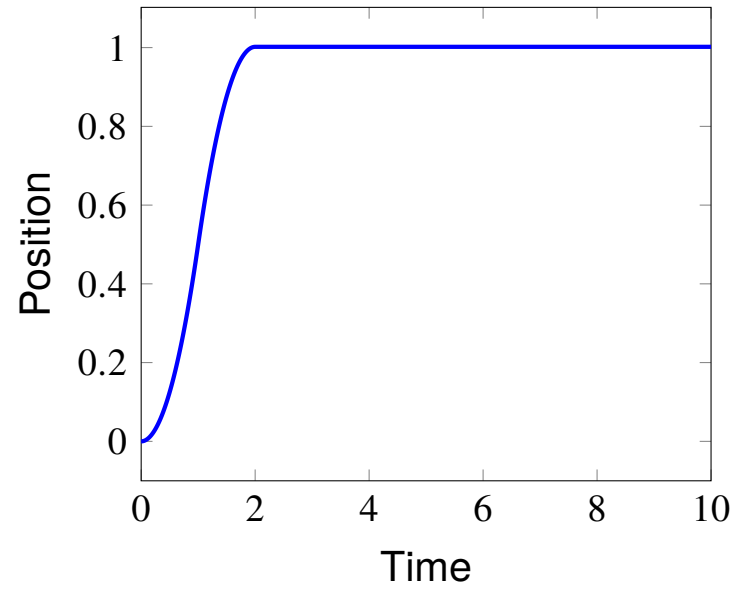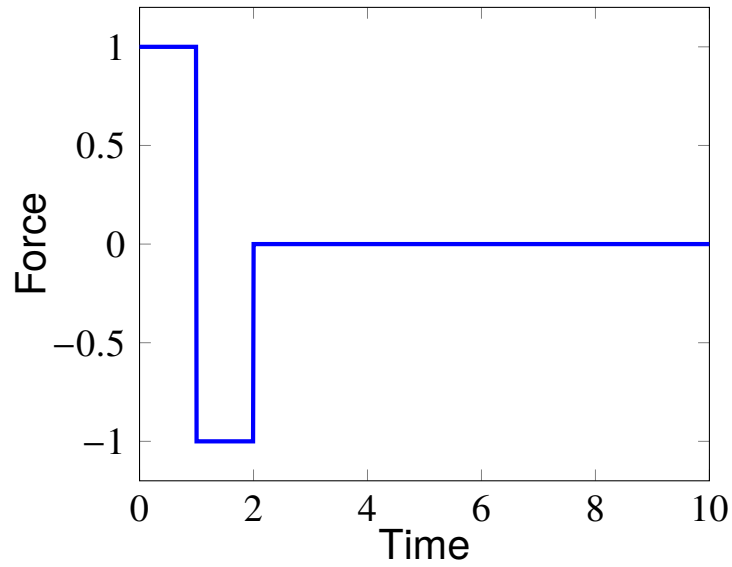- solutions with only two nonzero elements:

$$x = (1, -1, 0, \ldots, 0), \qquad x = (0, 1, -1, \ldots, 0), \qquad \ldots$$

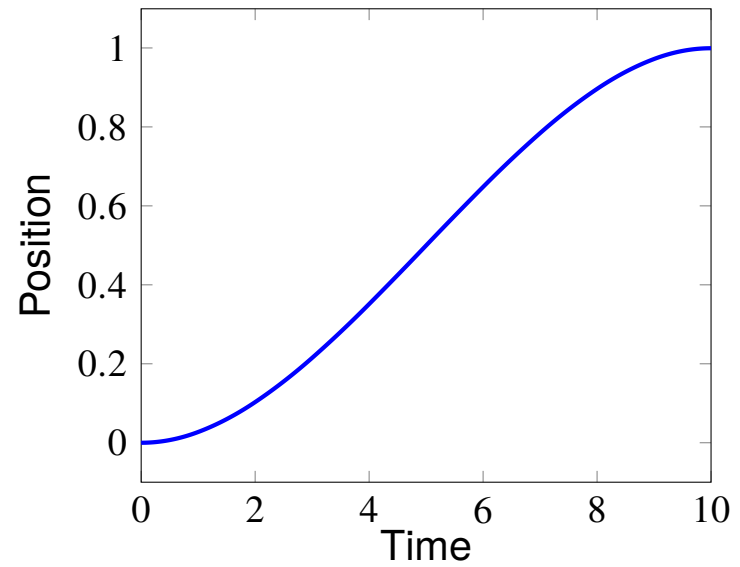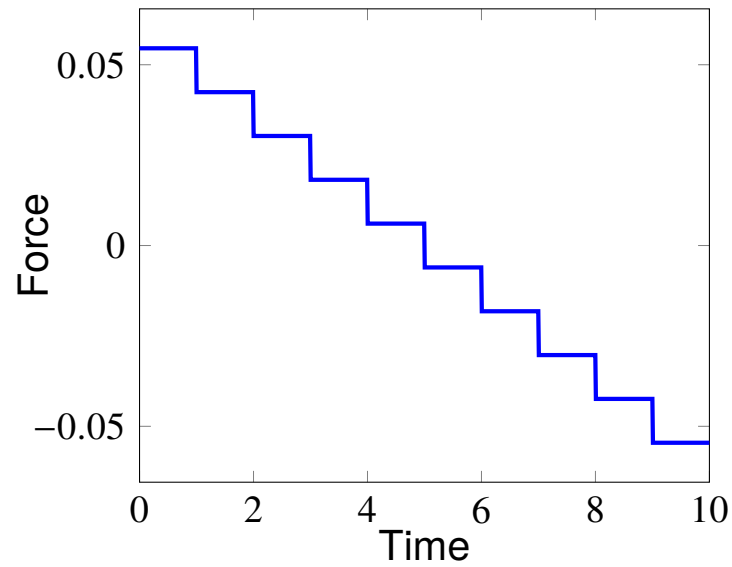- least norm solution: minimizes

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

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 $a \neq 0$:

$$\begin{array}{ll} \text{minimize} & \|x - a\|^2 \\ \text{subject to} & Cx = d \end{array}$$

- reduces to least norm problem by a change of variables $y = x - a$

$$\begin{array}{ll} \text{minimize} & \|y\|^2 \\ \text{subject to} & Cy = d - Ca \end{array}$$

- 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

$$
\begin{aligned}
\hat{x} &= C^T(CC^T)^{-1}d \\
&= C^\dagger d
\end{aligned}
$$

is the unique solution of the least norm problem

$$
\begin{array}{ll}
\text{minimize} & \|x\|^2 \\
\text{subject to} & Cx = d
\end{array}
$$

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

- recall from page 4.25 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 $x \neq \hat{x}$

$$
\begin{aligned}
\|x\|^2 &= \|\hat{x} + x - \hat{x}\|^2 \\
&= \|\hat{x}\|^2 + 2\hat{x}^T(x - \hat{x}) + \|x - \hat{x}\|^2 \\
&= \|\hat{x}\|^2 + \|x - \hat{x}\|^2 \\
&\geq \|\hat{x}\|^2
\end{aligned}
$$

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 $C^T = QR$ ($2p^2n$ flops)

2. solve $R^Tz = d$ by forward substitution (p^2 flops)

3. matrix-vector product $\hat{x} = Qz$ ($2pn$ flops)

complexity: $2p^2n$ flops

Example

$$C = \begin{bmatrix} 1 & -1 & 1 & 1 \\ 1 & 0 & 1/2 & 1/2 \end{bmatrix}, \qquad d = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

- QR factorization $C^T = QR$

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

- 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

$$\text{minimize} \quad \|Ax - b\|^2$$
$$\text{subject to} \quad Cx = d$$

- 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 $(x_1, y_1), \ldots, (x_N, y_N)$

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

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

two polynomials of degree 4

$g(x)$

$f(x)$

a
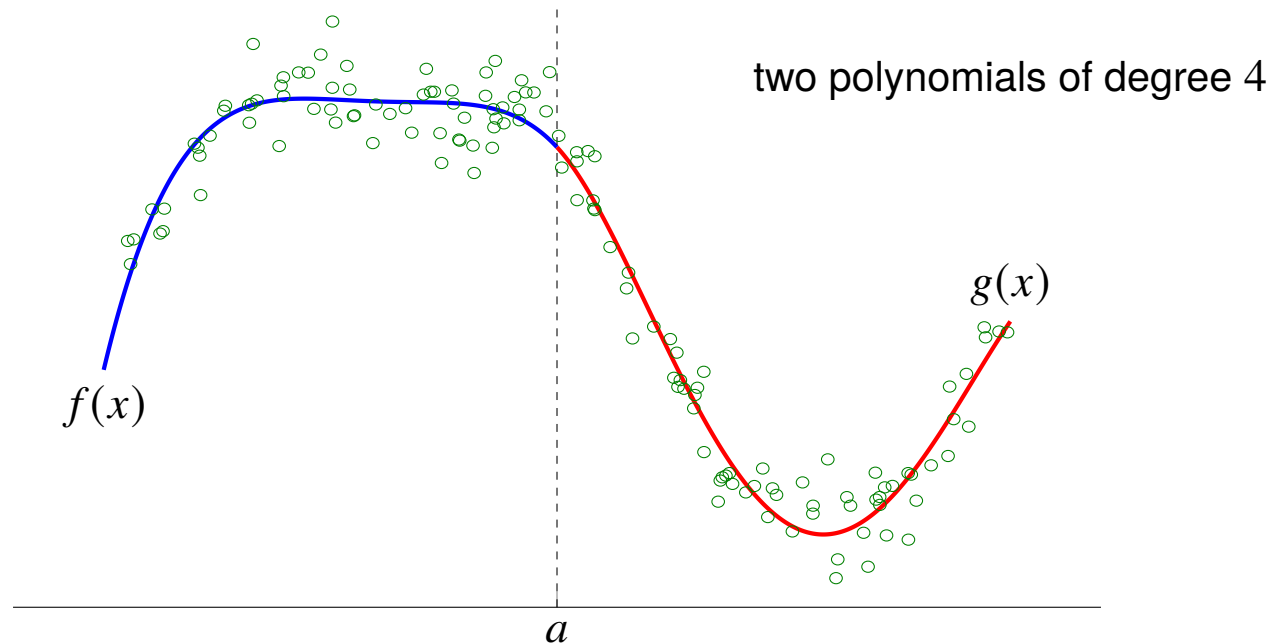
Constrained least squares formulation

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

$$\text{minimize} \quad \sum_{i=1}^{M} (f(x_i) - y_i)^2 + \sum_{i=M+1}^{N} (g(x_i) - y_i)^2$$

$$\text{subject to} \quad f(a) = g(a), \quad f'(a) = g'(a)$$

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

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

$$C = \begin{bmatrix} 1 & a & \cdots & a^{d-1} & -1 & -a & \cdots & -a^{d-1} \\ 0 & 1 & \cdots & (d-1)a^{d-2} & 0 & -1 & \cdots & -(d-1)a^{d-2} \end{bmatrix}, \qquad d = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Assumptions

$$\text{minimize} \quad \|Ax - b\|^2$$
$$\text{subject to} \quad Cx = d$$

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 $p \le n \le m + p$

Optimality conditions

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

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

(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 $A^T A \hat{x} = A^T b$

- 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

$$
\begin{aligned}
\|Ax - b\|^2 &= \|A(x - \hat{x}) + A\hat{x} - b\|^2 \\
&= \|A(x - \hat{x})\|^2 + \|A\hat{x} - b\|^2 + 2(x - \hat{x})^T A^T (A\hat{x} - b) \\
&= \|A(x - \hat{x})\|^2 + \|A\hat{x} - b\|^2 - 2(x - \hat{x})^T C^T z \\
&= \|A(x - \hat{x})\|^2 + \|A\hat{x} - b\|^2 \\
&\geq \|A\hat{x} - b\|^2
\end{aligned}
$$

- 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

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

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.

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

$$\implies \|Ax\|^2 = 0, \quad Cx = 0$$

$$\implies Ax = 0, \quad Cx = 0$$

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

if $x = 0$, we have $C^T z = -A^T Ax = 0$; 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 4.21)

- assumption 1 guarantees that the following QR factorization exists:

$$\begin{bmatrix} A \\ C \end{bmatrix} = QR = \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} R$$

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:

$$Q_2^T u = R^{-T} C^T u = 0 \quad \Longrightarrow \quad C^T u = 0 \quad \Longrightarrow \quad u = 0$$

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 simpflified 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

$$\begin{bmatrix} A \\ C \end{bmatrix} = \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} R, \qquad Q_2^T = \tilde{Q}\tilde{R}$$

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

$$mn^2 + \frac{2}{3}(p+n)^3 \leq mn^2 + \frac{16}{3}n^3 \quad \text{flops}$$

- QR factorization

$$2(p+m)n^2 + 2np^2 \leq 2mn^2 + 4n^3 \quad \text{flops}$$

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

$$x_{t+1} = A_t x_t + B_t u_t, \qquad y_t = C_t x_t, \qquad t = 1, 2, \ldots$$

- 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

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

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

$$x_1 = x^{\text{init}}, \qquad x_T = x^{\text{des}}$$

Linear quadratic control problem

minimize $\quad \|C_1 x_1\|^2 + \cdots + \|C_T x_T\|^2 + \rho(\|u_1\|^2 + \cdots + \|u_{T-1}\|^2)$

subject to $\quad x_{t+1} = A_t x_t + B_t u_t, \quad t = 1, \ldots, T-1$

$$x_1 = x^{\text{init}}, \quad x_T = x^{\text{des}}$$

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

Constrained least squares formulation

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

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

$$\tilde{A} = \left[\begin{array}{ccc|ccc} C_1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & C_T & 0 & \cdots & 0 \\ \hline 0 & \cdots & 0 & \sqrt{\rho}I & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & \cdots & \sqrt{\rho}I \end{array}\right], \qquad \tilde{b} = 0$$

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

$$\tilde{C} = \left[\begin{array}{cccccc|cccc} A_1 & -I & 0 & \cdots & 0 & 0 & B_1 & 0 & \cdots & 0 \\ 0 & A_2 & -I & \cdots & 0 & 0 & 0 & B_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & A_{T-1} & -I & 0 & 0 & \cdots & B_{T-1} \\ \hline I & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & I & 0 & 0 & \cdots & 0 \end{array}\right], \qquad \tilde{d} = \left[\begin{array}{c} 0 \\ 0 \\ \vdots \\ 0 \\ \hline x^{\text{init}} \\ x^{\text{des}} \end{array}\right]$$

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)

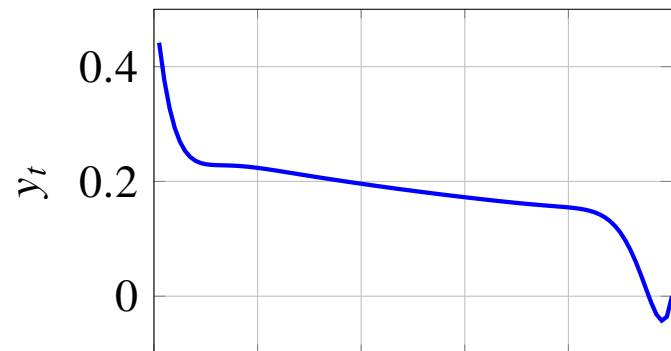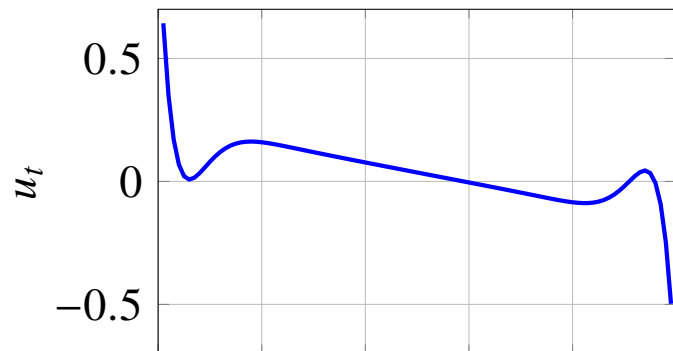- figure shows "open-loop" output $CA^{t-1}x^{\text{init}}$
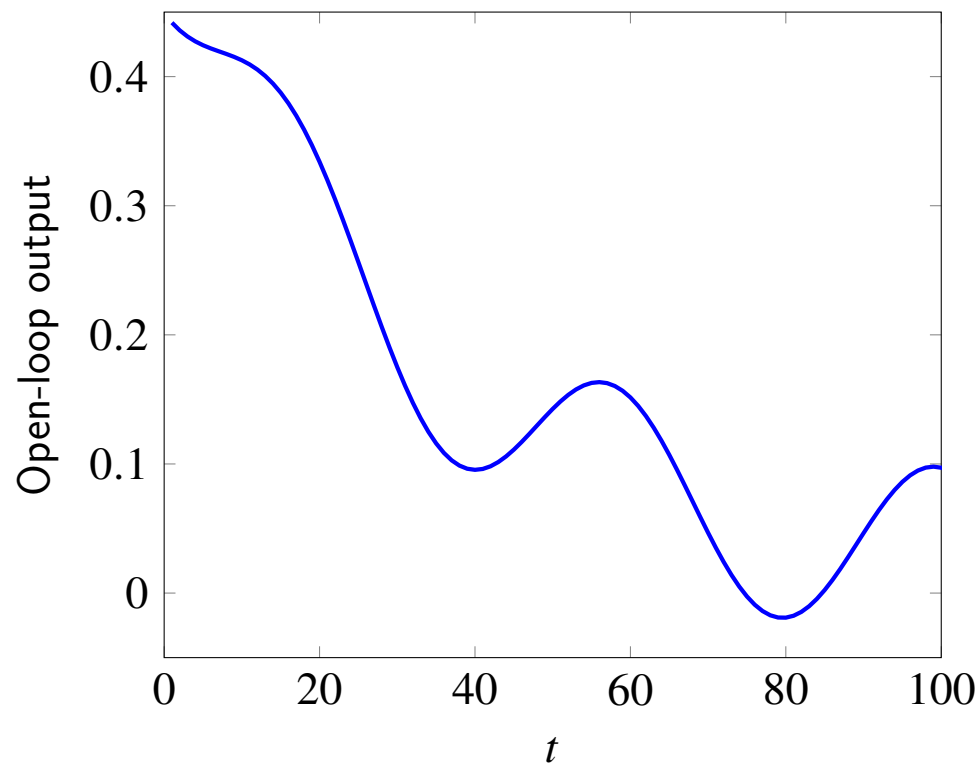
- we minimize $J_{\text{output}} + \rho J_{\text{input}}$ with final state constraint $x^{\text{des}} = 0$ at $T = 100$
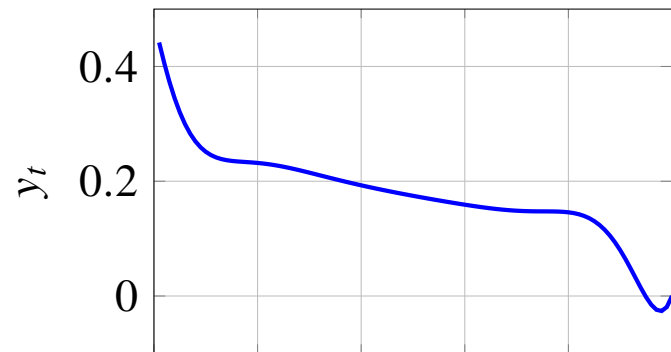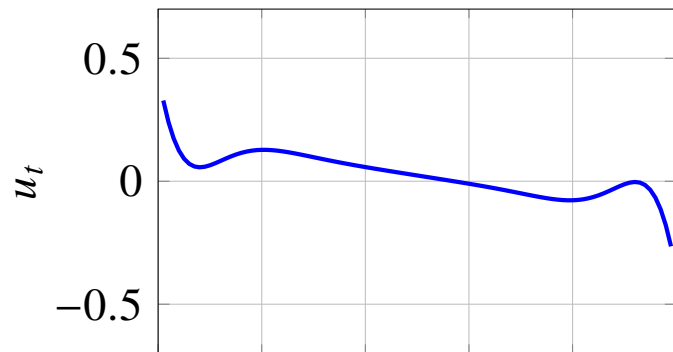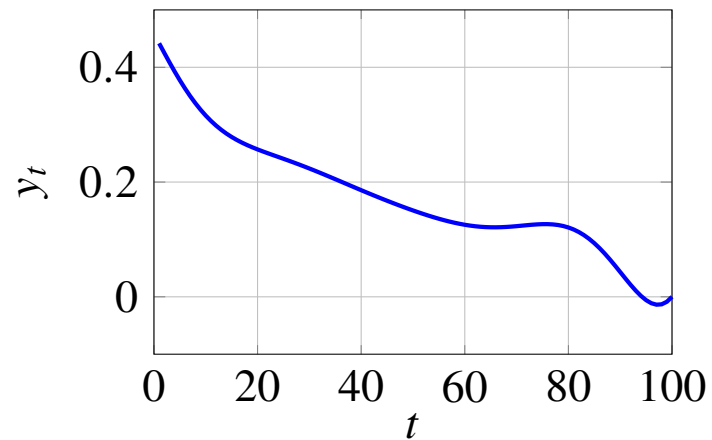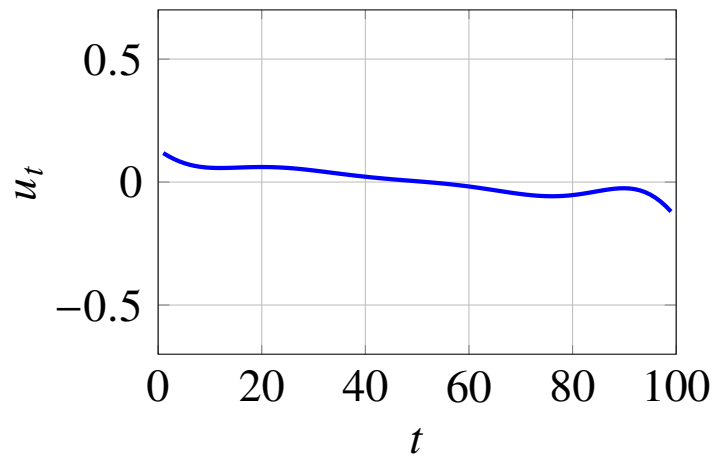
Optimal trade-off curve
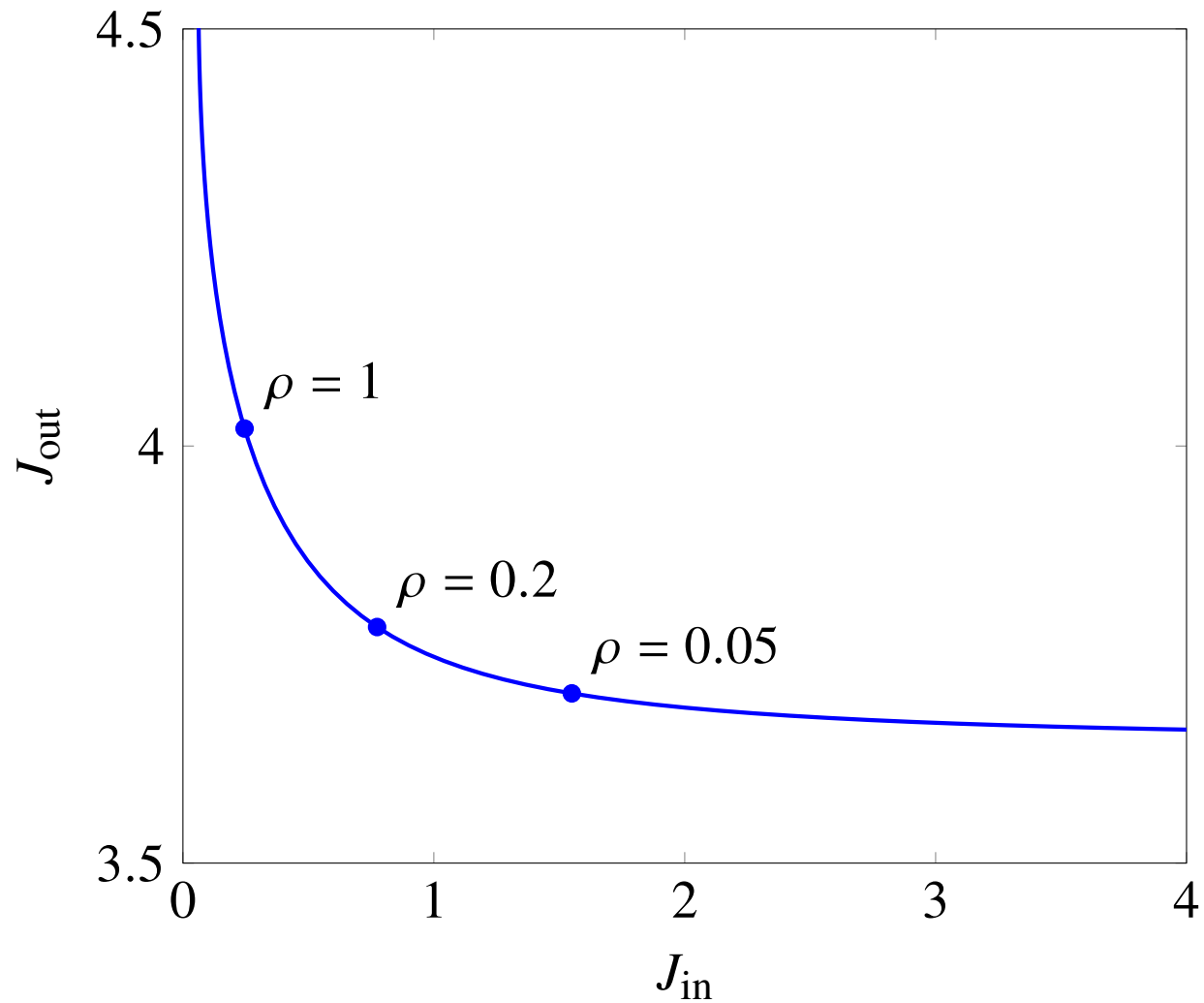
Three solutions on the trade-off curve

$\rho = 0.05$

$\rho = 0.2$

$\rho = 1$

Linear state feedback control

Linear state feedback
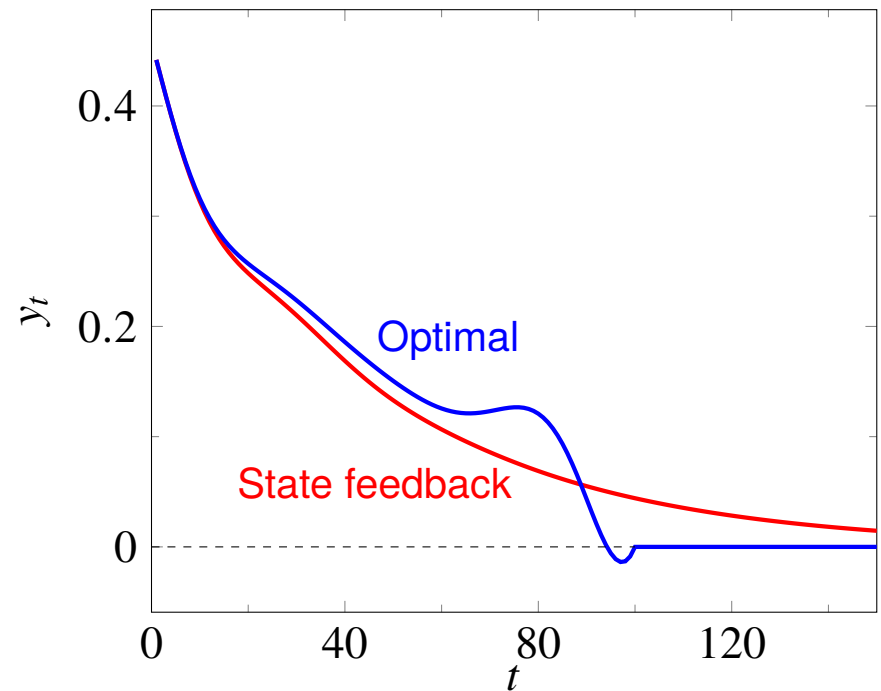
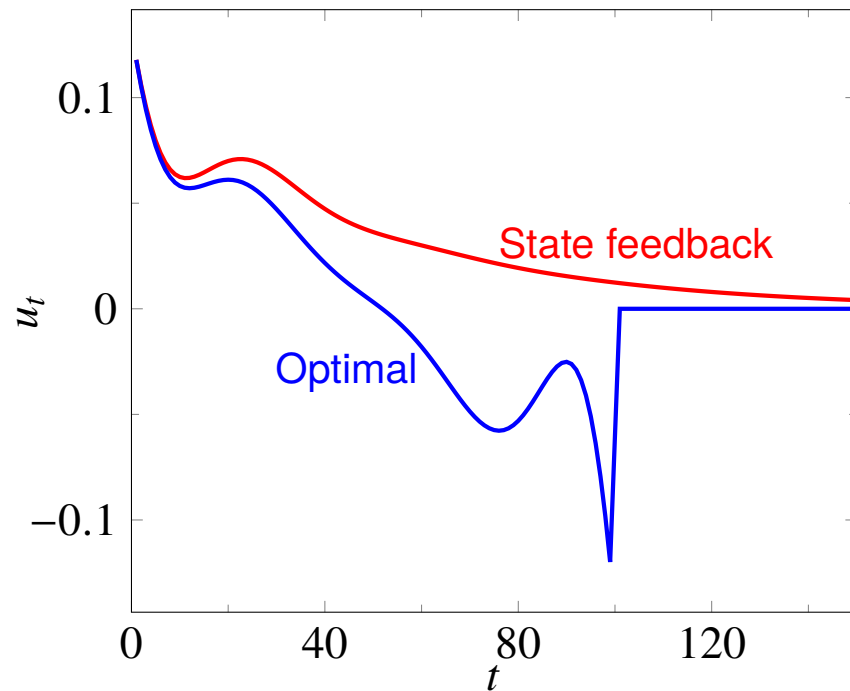- linear state feedback control uses the input

$$u_t = Kx_t, \quad t = 1, 2, \ldots$$

- 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^{init}, hence u_1 can be written as $u_1 = Kx^{\text{init}}$

- 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

Example

- system matrices of previous example

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

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