Constrained Least Squares

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Outline

Linearly constrained least squares

Least norm problem

Solving the constrained least squares problem

Least squares with equality constraints

- the (linearly) *constrained least squares problem* (CLS) is

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

- variable (to be chosen/found) is n-vector x
- $m \times n$ matrix A, m-vector b, $p \times n$ matrix C, and p-vector d are *problem data* (*i.e.*, they are given)
- $\|Ax - b\|^2$ is the *objective function*
- $Cx = d$ are the *equality constraints*
- x is *feasible* if $Cx = d$
- $\hat{x}$ is a *solution* of CLS if $C\hat{x} = d$ and $\|A\hat{x} - b\|^2 \leq \|Ax - b\|^2$ holds for any n-vector x that satisfies $Cx = d$

Least squares with equality constraints

- CLS combines solving linear equations with least squares problem
- like a bi-objective least squares problem, with infinite weight on second objective $\|Cx - d\|^2$

Piecewise-polynomial fitting

- *piecewise-polynomial* $\hat{f}$ has form

$$\hat{f}(x) = \begin{cases} p(x) = \theta_1 + \theta_2 x + \theta_3 x^2 + \theta_4 x^3 & x \leq a \\ q(x) = \theta_5 + \theta_6 x + \theta_7 x^2 + \theta_8 x^3 & x > a \end{cases}$$

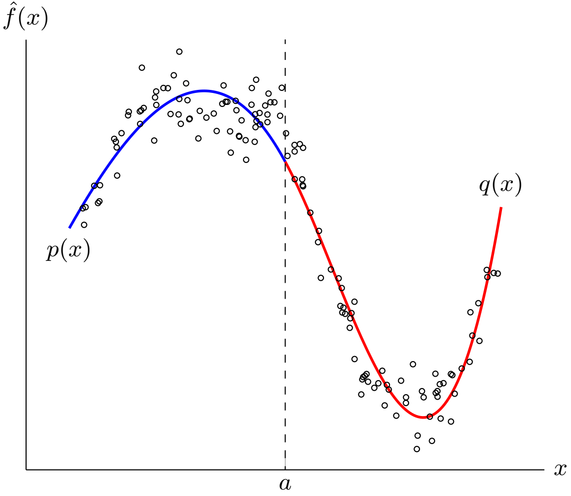
  (a is given)

- we require $p(a) = q(a)$, $p'(a) = q'(a)$
- fit $\hat{f}$ to data (x_i, y_i), $i = 1, \ldots, N$ by minimizing sum square error

$$\sum_{i=1}^{N} (\hat{f}(x_i) - y_i)^2$$

- can express as a constrained least squares problem

Example



Piecewise-polynomial fitting

- constraints are (linear equations in θ)

$$\begin{aligned}\theta_1 + \theta_2 a + \theta_3 a^2 + \theta_4 a^3 - \theta_5 - \theta_6 a - \theta_7 a^2 - \theta_8 a^3 &= 0 \\ \theta_2 + 2\theta_3 a + 3\theta_4 a^2 - \theta_6 - 2\theta_7 a - 3\theta_8 a^2 &= 0\end{aligned}$$

- prediction error on (x_i, y_i) is $a_i^T\theta - y_i$, with

$$(a_i)_j = \begin{cases} (1, x_i, x_i^2, x_i^3, 0, 0, 0, 0) & x_i \le a \\ (0, 0, 0, 0, 1, x_i, x_i^2, x_i^3) & x_i > a \end{cases}$$

- sum square error is $\|A\theta - y\|^2$, where a_i^T are rows of A

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Least norm problem

- special case of constrained least squares problem, with $A = I$, $b = 0$
- *least-norm problem*:

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

i.e., find the smallest vector that satisfies a set of linear equations

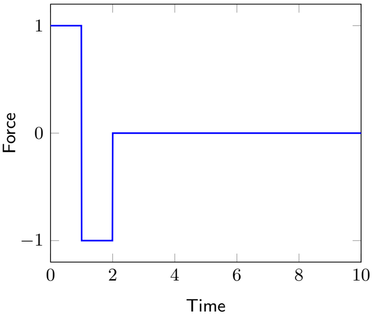
Force sequence

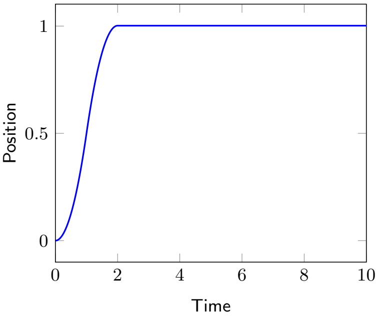
- unit mass on frictionless surface, initially at rest
- 10-vector f gives forces applied for one second each
- final velocity and position are

$$\begin{aligned} v^{\rm fin} &= f_1 + f_2 + \cdots + f_{10} \\ p^{\rm fin} &= (19/2)f_1 + (17/2)f_2 + \cdots + (1/2)f_{10} \end{aligned}$$

- let's find f for which $v^{\rm fin} = 0$, $p^{\rm fin} = 1$
- $f^{\rm bb} = (1, -1, 0, \ldots, 0)$ works (called 'bang-bang')

Bang-bang force sequence





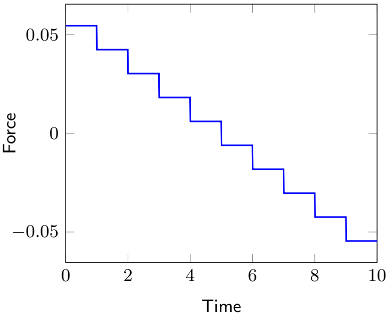
Least norm force sequence

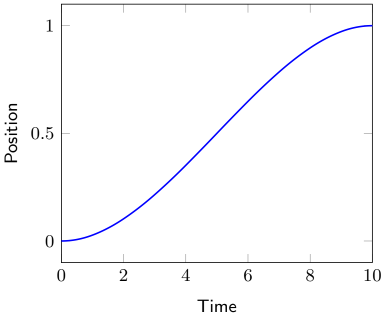
- let's find least-norm f that satisfies $p^{\text{fin}} = 1$, $v^{\text{fin}} = 0$
- least-norm problem:

$$\begin{array}{ll} \text{minimize} & \|f\|^2 \\ \text{subject to} & \left[\begin{array}{ccccc} 1 & 1 & \cdots & 1 & 1 \\ 19/2 & 17/2 & \cdots & 3/2 & 1/2 \end{array}\right] f = \left[\begin{array}{c} 0 \\ 1 \end{array}\right] \end{array}$$

  with variable f
- solution f^{ln} satisfies $\|f^{\text{ln}}\|^2 = 0.0121$ (compare to $\|f^{\text{bb}}\|^2 = 2$)

Least norm force sequence





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Optimality conditions via calculus

to solve constrained optimization problem

$$\begin{array}{ll} \text{minimize} & f(x) = \|Ax - b\|^2 \\ \text{subject to} & c_i^T x = d_i, \quad i = 1, \ldots, p \end{array}$$

1. form *Lagrangian* function, with *Lagrange multipliers* $z_1, \ldots, z_p$

$$L(x, z) = f(x) + z_1(c_1^T x - d_1) + \cdots + z_p(c_p^T x - d_p)$$

2. optimality conditions are

$$\frac{\partial L}{\partial x_i}(\hat{x}, z) = 0, \quad i = 1, \ldots, n, \qquad \frac{\partial L}{\partial z_i}(\hat{x}, z) = 0, \quad i = 1, \ldots, p$$

Optimality conditions via calculus

- $\dfrac{\partial L}{\partial z_i}(\hat{x}, z) = c_i^T \hat{x} - d_i = 0$, which we already knew
- first n equations are more interesting:

$$\frac{\partial L}{\partial x_i}(\hat{x}, z) = 2\sum_{j=1}^{n}(A^TA)_{ij}\hat{x}_j - 2(A^Tb)_i + \sum_{j=1}^{p} z_j c_i = 0$$

- in matrix-vector form: $2(A^TA)\hat{x} - 2A^Tb + C^Tz = 0$
- put together with $C\hat{x} = d$ to get *KKT conditions*

$$\left[\begin{array}{cc} 2A^TA & C^T \\ C & 0 \end{array}\right]\left[\begin{array}{c} \hat{x} \\ z \end{array}\right] = \left[\begin{array}{c} 2A^Tb \\ d \end{array}\right]$$

  a square set of $n+p$ linear equations in variables $\hat{x}$, z
- KKT equations are extension of normal equations to CLS

Solution of constrained least squares problem

- assuming the KKT matrix is invertible, we have

$$\begin{bmatrix} \hat{x} \\ z \end{bmatrix} = \begin{bmatrix} 2A^TA & C^T \\ C & 0 \end{bmatrix}^{-1} \begin{bmatrix} 2A^Tb \\ d \end{bmatrix}$$

- KKT matrix is invertible if and only if

$$C \textit{ has independent rows, and } \begin{bmatrix} A \\ C \end{bmatrix} \textit{ has independent columns}$$

- implies $m + p \geq n$, $p \leq n$
- can compute $\hat{x}$ in $2mn^2 + 2(n+p)^3$ flops; order is n^3 flops

Direct verification of solution

- to show that $\hat{x}$ is solution, suppose x satisfies $Cx = d$
- then

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

- expand last term, using $2A^T(A\hat{x} - b) = -C^T z$, $Cx = C\hat{x} = d$:

$$\begin{aligned} 2(Ax - A\hat{x})^T(A\hat{x} - b) &= 2(x - \hat{x})^T A^T (A\hat{x} - b) \\ &= -(x - \hat{x})^T C^T z \\ &= -(C(x - \hat{x}))^T z \\ &= 0 \end{aligned}$$

- so $\|Ax - b\|^2 = \|A(x - \hat{x})\|^2 + \|A\hat{x} - b\|^2 \geq \|A\hat{x} - b\|^2$
- and we conclude $\hat{x}$ is solution

Solution of least-norm problem

- least-norm problem: minimize $\|x\|^2$ subject to $Cx = d$
- matrix $\begin{bmatrix} I \\ C \end{bmatrix}$ always has independent columns
- we assume that C has independent rows
- optimality condition reduces to

$$\begin{bmatrix} 2I & C^T \\ C & 0 \end{bmatrix} \begin{bmatrix} \hat{x} \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ d \end{bmatrix}$$

- so $\hat{x} = -(1/2)C^T z$; second equation is then $-(1/2)CC^T z = d$
- plug $z = -2(CC^T)^{-1}d$ into first equation to get

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

where $C^\dagger$ is (our old friend) the pseudo-inverse so when C has independent rows:

- $C^\dagger$ is a right inverse of C
- so for any d, $\hat{x} = C^\dagger d$ satisfies $C\hat{x} = d$
- and we now know: $\hat{x}$ is the *smallest* solution of $Cx = d$