Explicit formula for Constrained Least Squares

Bill Menke, July 21, 2023

Although I allude to this formula in the Fourth Edition of Geophysical Data Analysis: Discrete Inverse Theory, I do not actually state it. I'm putting it in the Fifth Edition, so here it is.

The problem is to minimize the L_2 error of $\mathbf{Gm} = \mathbf{d}$ with the hard constraint that $\mathbf{Hm} = \mathbf{h}$. In the book, I show that this leads to the Lagrange equation:

$$\begin{bmatrix} \mathbf{G}^T\mathbf{G} & \mathbf{H}^T \\ \mathbf{H} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{m} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \mathbf{G}^T\mathbf{d} \\ \mathbf{h} \end{bmatrix}$$

Where $\boldsymbol{\lambda}$ is a vector of Lagrange multipliers. I advocate simply solving this equation directly for $[\mathbf{m}, \boldsymbol{\lambda}]^T$ and then discarding the $\boldsymbol{\lambda}$ However, it does have an explicit solution for $\mathbf{m}$.

Wikipedia (https://en.wikipedia.org/wiki/Block_matrix) gives the inverse of a 2×2 block matrix as:

$$\mathbf{P} = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{A}^{-1} + \mathbf{A}^{-1}\mathbf{B}(\mathbf{D} - \mathbf{C}\mathbf{A}^{-1}\mathbf{B})^{-1}\mathbf{C}\mathbf{A}^{-1} & -\mathbf{A}^{-1}\mathbf{B}(\mathbf{D} - \mathbf{C}\mathbf{A}^{-1}\mathbf{B})^{-1} \\ -(\mathbf{D} - \mathbf{C}\mathbf{A}^{-1}\mathbf{B})^{-1}\mathbf{C}\mathbf{A}^{-1} & (\mathbf{D} - \mathbf{C}\mathbf{A}^{-1}\mathbf{B})^{-1} \end{bmatrix},$$

For the over-determined case, the Gram matrix, $\mathbf{G}^T\mathbf{G}$, is invertible and the above formula can be applied. Comparing terms:

$$\mathbf{P}_{11} = [\mathbf{G}^T\mathbf{G}]^{-1} - [\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{H}^T(\mathbf{H}[\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{H}^T)^{-1}\mathbf{H}[\mathbf{G}^T\mathbf{G}]^{-1}$$

$$\mathbf{P}_{12} = [\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{H}^T[\mathbf{G}^T\mathbf{G}]^{-1}(\mathbf{H}[\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{H}^T)^{-1}$$

$$\mathbf{m} = \mathbf{P}_{11}\mathbf{G}^T\mathbf{d} + \mathbf{P}_{12}\mathbf{h}$$

$$= [\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{G}^T\mathbf{d} - [\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{H}^T(\mathbf{H}[\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{H}^T)^{-1}\mathbf{H}[\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{G}^T\mathbf{d}$$
$$+ [\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{H}[\mathbf{G}^T\mathbf{G}]^{-1}(\mathbf{H}[\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{H}^T)^{-1}\mathbf{h}$$

$$= \mathbf{m}_{LS} - [\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{H}^T(\mathbf{H}[\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{H}^T)^{-1}\mathbf{H}\mathbf{m}_{LS} + [\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{H}[\mathbf{G}^T\mathbf{G}]^{-1}(\mathbf{H}[\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{H}^T)^{-1}\mathbf{h}$$

$$\mathbf{m}_{LS} + [\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{H}^T(\mathbf{H}[\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{H}^T)^{-1}(\mathbf{h} - \mathbf{H}\mathbf{m}_{LS})$$

with least squares solution $\mathbf{m}_{LS} \equiv [\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{G}^T\mathbf{d}$. Note that the second term on the r.h.s. contains a correction to the least squares solution whose amplitude depends on the misfit between the prior information, $\mathbf{h}$, and the value, $\mathbf{H}\mathbf{m}_{LS}$, predicted by the least squares solution.

Example: Constrained fitting of a straight line, in which the line is constrained to pass through a specified point.

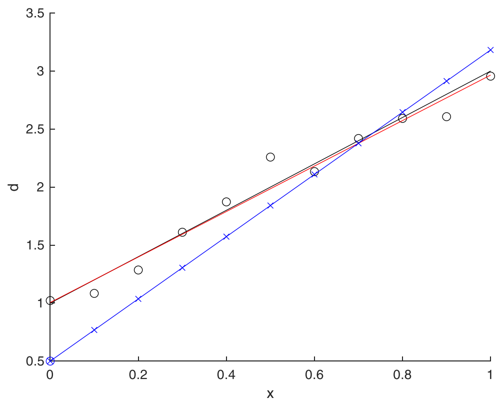

Fig. 1. Plot of $d(x)$ for the model $d(x_i) = m_1 + m_2 x_i$. True data (black line), noisy observed data (black circles), constraint point $(x_0, d_0) = (0.0, 0.5\ )$ (blue circle), constrained fit solving Lagrange equation directly (blue line), constrained fit solving Lagrange equation explicitly (blue crosses). Note that direct and explicit solutions are equal.

In most instances, the direct solution of the Lagrange equation is preferable, because one can exploits any sparseness in its component parts, $\mathbf{G}^T\mathbf{G}$ and $\mathbf{H}$.

Exemplary MATLAB® code

```
clear all;
N=11;
x = [0:N-1]'/(N-1);
G = [ ones(N,1), x];
GTG = G'*G;
GTGI = inv(GTG);
mtrue=[1,2]';
dtrue = G*mtrue;
sigmad=0.1;
dobs = dtrue + random('Normal',0, sigmad,N,1);
GTd = G'*dobs;
mls = GTG\GTd;
x0 = 0.0;
d0 = 0.5;
figure();
clf;
hold on;
plot(x,dtrue,'k-');
plot(x,dobs,'ko');
plot(x0,d0,'bo');
xlabel('x');
ylabel('d');
```

```
H = [1,x0];
h = [d0];
M = [GTG, H'; H, 0];
z = [GTd; h];
y = M\z;
mest = y(1:2);
dpre = G*mest;
plot(x,dpre,'b-');
Z = H*GTGI*H';
ZI = inv(Z);
mnew = mls + GTGI*H'*ZI*(h-H*mls);
dnew = G*mnew;
plot(x,dpre,'bx');
```