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Solution of overdetermined systems

Consider an overdetermined linear system:

$$Ax = b,$$

where $A \in \mathbb{R}^{m \times n}$, $m \geq n$, and $b \in \mathbb{R}^m$. We assume that $A$ has a full column rank, $\text{rank}(A) = n$. In this setting, the system is usually inconsistent (has no solution) and a common approach for finding an approximate solution is to

$$(LS) : \min_{x \in \mathbb{R}^n} \|Ax - b\|^2,$$

or equivalently, to

$$(LS) : \min_{x \in \mathbb{R}^n} \left\{ f(x) := x^\top (A^\top A)x - 2(A^\top b)^\top x + \|b\|^2 \right\}.$$

Since $A$ is of full column rank, $\nabla^2 f(x) = 2A^\top A \succ 0$, $\forall x \in \mathbb{R}^n$. Therefore, (by Lemma 2.41), the unique stationary point

$$x_{LS} = (A^\top A)^{-1}A^\top b$$

is the optimal solution of problem (LS), and $x_{LS}$ is called the least squares solution of the system $Ax = b$. 

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The normal system

- It is quite common not to write the explicit expression for $x_{LS}$ but instead to write the associated system of equations that defines it:

$$ (A^T A)x_{LS} = A^T b. $$

The above system of equations is called the normal system.

- If $m = n$ and $A$ is of full column rank, then $A$ is nonsingular. In this case, the least squares solution is actually the solution of the linear system $Ax = b$, since

$$ x_{LS} = (A^T A)^{-1} A^T b = A^{-1} A^{-T} A^T b = A^{-1} b = x. $$
Example

Consider the inconsistent linear system

\[ Ax = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix} = b. \]

The least squares problem can be explicitly written as

\[
\min_{(x_1, x_2) \in \mathbb{R}^2} \left\{ (x_1 + 2x_2)^2 + (2x_1 + x_2 - 1)^2 + (3x_1 + 2x_2 - 1)^2 \right\}.
\]

We will solve the normal equations:

\[
\begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 2 \end{bmatrix}^\top \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 2 \end{bmatrix}^\top \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix},
\]

which are the same as

\[
\begin{bmatrix} 14 & 10 \\ 10 & 9 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 5 \\ 3 \end{bmatrix}.
\]
The solution of the above system is the least squares estimate

\[ x_{LS} = \begin{bmatrix} 15/26 \\ -8/26 \end{bmatrix}. \]

The residual vector is given by

\[ r := Ax_{LS} - b = \begin{bmatrix} -0.038 \\ -0.154 \\ 0.115 \end{bmatrix}, \]

and \( \|r\|_2^2 = (-0.038)^2 + (-0.154)^2 + (0.115)^2 \approx 0.038. \)

To find the least squares solution in MATLAB:

\[
\begin{align*}
&\text{>> } A = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 2 \end{bmatrix}; \\
&\text{>> } b = \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}; \\
&\text{>> } \text{format rational;} \\
&\text{>> } A\backslash b \\
&\text{ans =} \\
&\quad 15/26 \\
&\quad -4/13
\end{align*}
\]
Data fitting: linear fitting

Suppose that we are given a set of data points \((s_i, t_i), i = 1, 2, \cdots, m, \)
\(s_i \in \mathbb{R}^n\) and \(t_i \in \mathbb{R}\,\), and assume that a linear relation of the form

\[
t_i = s_i^\top x, \quad i = 1, 2, \cdots, m,
\]

approximately holds. The objective is to find the parameters vector \(x \in \mathbb{R}^n\). The least squares approach is to

\[
\min_{x \in \mathbb{R}^n} \sum_{i=1}^{m} (s_i^\top x - t_i)^2.
\]

We can alternatively write the problem as

\[
\min_{x \in \mathbb{R}^n} \|Sx - t\|^2,
\]

where

\[
S = \begin{bmatrix} s_1^\top \\ s_2^\top \\ \vdots \\ s_m^\top \end{bmatrix}, \quad t = \begin{bmatrix} t_1 \\ t_2 \\ \vdots \\ t_m \end{bmatrix}.
\]
Example

Consider 30 points in $\mathbb{R}^2$, $x_i = (i - 1)/29$, $y_i = 2x_i + 1 + \varepsilon_i$, for $i = 1, 2, \cdots, 30$, where $\varepsilon_i$ is randomly generated from a standard normal distribution $\mathcal{N}(0, (0.1)^2)$. The objective is to find a line of the form $y = ax + b$ that best fits them. The corresponding linear system that needs to be “solved” is

$$
\begin{bmatrix}
x_1 & 1 \\
x_2 & 1 \\
\vdots & \vdots \\
x_{30} & 1
\end{bmatrix}
\begin{bmatrix}
a \\
b
\end{bmatrix}
=
\begin{bmatrix}
y_1 \\
y_2 \\
\vdots \\
y_{30}
\end{bmatrix}.
$$

The least squares solution is $(a, b)^\top = (X^\top X)^{-1}X^\top y$.

```matlab
randn('seed', 319);
d = linspace(0, 1, 30));
e = 2*d + 1 + 0.1*randn(30, 1);
plot(d, e, 'r*')
```
Example (cont’d)

```matlab
>> u = [d, ones(30, 1)]
>> a = u(1), b = u(2)
    a =
    2.0616
    b =
    0.9725
```

Note that the obtained estimates of $a$ and $b$ are very close to the “true” $a$ and $b$ (2 and 1, respectively) that were used to generate the data. The least squares line as well as the 30 points is described in the right image of Figure 3.1.

The least squares approach can be used also in nonlinear fitting. Suppose, for example, that we are given a set of points in $\mathbb{R}^2$: $(u_i, y_i)$, $i = 1, 2, \ldots, m$, and that we know a priori that these points are approximately related via a polynomial of degree at most $d$; i.e., there exists $a_0, \ldots, a_d$ such that

$$d \sum_{j=0}^{d} a_j u_j^i \approx y_i, \quad i = 1, \ldots, m.$$ 

The least squares approach to this problem seeks $a_0, a_1, \ldots, a_d$ that are the least squares solution to the linear system

$$
\begin{bmatrix}
1 & u_1 & u_2 & \cdots & u_d \\
1 & u_2 & u_2 & \cdots & u_d \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
1 & u_m & u_d & \cdots & u_d
\end{bmatrix}
\begin{bmatrix}
a_0 \\
a_1 \\
\vdots \\
a_d
\end{bmatrix}
=
\begin{bmatrix}
y_0 \\
y_1 \\
\vdots \\
y_m
\end{bmatrix}.
$$

The least squares solution is of course well-defined if the $m \times (d + 1)$ matrix is of a full column rank. This of course suggests in particular that $m \geq d + 1$. The matrix $U$ consists
Nonlinear fitting

Suppose that we are given a set of points in \( \mathbb{R}^2 \), \((u_i, y_i)\), \(1 \leq i \leq m\), \(u_i \neq u_j\) for \(i \neq j\), and that we know a priori that these points are approximately related via a polynomial of degree at most \(d\) and \(m \geq d + 1\), i.e., \(\exists a_0, a_1, \ldots, a_d\) such that

\[
\sum_{j=0}^{d} a_j u_i^j \approx y_i, \quad i = 1, 2, \ldots, m.
\]

The least squares approach to this problem seeks \(a_0, a_1, \ldots, a_d\) that are the least squares solution to the linear system

\[
\begin{bmatrix}
1 & u_1 & u_1^2 & \cdots & u_1^d \\
1 & u_2 & u_2^2 & \cdots & u_2^d \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
1 & u_m & u_m^2 & \cdots & u_m^d 
\end{bmatrix}_{m \times (d+1)} \begin{bmatrix}
a_0 \\
a_1 \\
\vdots \\
a_d 
\end{bmatrix}_{(d+1) \times 1} = \begin{bmatrix}
y_0 \\
y_1 \\
\vdots \\
y_m 
\end{bmatrix}_{(d+1) \times 1}.
\]

\(\begin{bmatrix}
1 & u_1 & u_1^2 & \cdots & u_1^d \\
1 & u_2 & u_2^2 & \cdots & u_2^d \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
1 & u_m & u_m^2 & \cdots & u_m^d 
\end{bmatrix}_{m \times (d+1)} : = U_{d+1}
\]

The matrix \(U_{d+1}\) is of a full column rank since it consists of the first \(d + 1\) columns of the so-called \(m \times m\) Vandermonde matrix which is nonsingular, \(\det(U_m) = \prod_{1 \leq i < j \leq m} (u_j - u_i) \neq 0\).
The regularized least squares (RLS) problem has the form

\[
(RLS) : \min_{x \in \mathbb{R}^n} \left\{ \|Ax - b\|^2 + \lambda R(x) \right\}.
\]

The positive constant \( \lambda \) is the regularization parameter. In many cases, the regularization is taken to be quadratic. In particular, \( R(x) = \|Dx\|^2 \), where \( D \in \mathbb{R}^{p \times n} \) is a given matrix. Then we have

\[
\min_{x \in \mathbb{R}^n} \left\{ f_{RLS}(x) := x^\top (A^\top A + \lambda D^\top D)x - 2(A^\top b)^\top x + \|b\|^2 \right\}.
\]

Since the Hessian of the objective function is

\[
\nabla^2 f_{RLS}(x) = 2(A^\top A + \lambda D^\top D) \succeq 0,
\]

any stationary point is a global minimum point (cf. Theorem 2.38). The stationary points are those satisfying \( \nabla f(x) = 0 \), that is

\[
(A^\top A + \lambda D^\top D)x = A^\top b.
\]

Therefore, if \( A^\top A + \lambda D^\top D \succeq 0 \) then the RLS solution is given by

\[
x_{RLS} = (A^\top A + \lambda D^\top D)^{-1}A^\top b.
\]
Let $A \in \mathbb{R}^{3 \times 3}$ be given by

\[
A = \begin{bmatrix}
2 + 10^{-3} & 3 & 4 \\
3 & 5 + 10^{-3} & 7 \\
4 & 7 & 10 + 10^{-3}
\end{bmatrix}.
\]

B = [1, 1, 1; 1, 2, 3];
A=B'*B + 0.001*eye(3);  \% cond(A) \approx 16000 is rather large!

The “true” vector was chosen to be $x_{true} = (1, 2, 3)^T$, and $b$ is a noisy measurement of $Ax_{true}$:

\[
\begin{align*}
\text{>> } & x_{true} = [1; 2; 3]; \\
\text{>> } & \text{randn('seed', 315);} \\
\text{>> } & b = A*x_{true} + 0.01*randn(3, 1) \\
& b = \\
& \begin{bmatrix}
20.0019 \\
34.0004 \\
48.0202
\end{bmatrix}
\end{align*}
\]

The relative perturbation on the RHS $b_{true}(:= Ax_{true})$ is not too small!
The matrix $A$ is in fact of a full column rank since its eigenvalues are all positive ($\text{eig}(A)$). The least squares solution $x_{LS}$ is given by

\[
\begin{bmatrix}
4.5446 \\
-5.1295 \\
6.5742
\end{bmatrix}
\]

Note that $x_{LS}$ is rather far from the true vector $x_{true}$. We will add the quadratic regularization function $\|Ix\|^2$. The regularized solution is

\[
x_{RLS} = (A^\top A + \lambda I)^{-1}A^\top b.
\]

\[
\begin{bmatrix}
1.1763 \\
2.0318 \\
2.8872
\end{bmatrix}
\]

which is a much better estimate for $x_{true}$ than $x_{LS}$. 

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Suppose that a noisy measurement of a signal $x \in \mathbb{R}^n$ is given

$$b = x + w,$$

where $x$ is an unknown signal, $w$ is an unknown noise vector, and $b$ is the known measurement vector. The denoising problem is to find a “good” estimate of $x$. The associated least squares problem is

$$\min_{x \in \mathbb{R}^n} \|x - b\|^2.$$

The optimal solution of this problem is obviously $x = b$, which is meaningless. We will add a regularization term $\lambda \sum_{i=1}^{n-1} (x_i - x_{i+1})^2$,

$$\min_{x \in \mathbb{R}^n} \left\{ \|Ix - b\|^2 + \lambda \|Lx\|^2 \right\},$$

where parameter $\lambda > 0$ and $L \in \mathbb{R}^{(n-1) \times n}$ is given by

$$L := \begin{bmatrix} 1 & -1 & 1 & -1 & \cdots & 1 & -1 \end{bmatrix}.$$ 

The optimal solution is given by $x_{RLS}(\lambda) = (I + \lambda L^\top L)^{-1}b$. 
Example

Consider the signal \( x \in \mathbb{R}^{300} \) constructed by

\[
t = \text{linspace}(0, 4, 300)';
x = \sin(t) + t.*(\cos(t).^2);
\]

\[
\text{randn('seed', 314)};
b = x + 0.05*\text{randn}(300, 1);
\]

subplot(1, 2, 1);
plot(1:300, x, 'LineWidth', 2);
subplot(1, 2, 2);
plot(1:300, b, 'LineWidth', 2);

---

Figure 3.2. A signal (left image) and its noisy version (right image).
Example (cont’d): \( \lambda = 1, 10, 100, 1000 \)

![Graphs showing different reconstructions with varying \( \lambda \) values.](image)

**signal \( x \):** marked with red dot
Nonlinear least squares

Suppose that we are given a system of nonlinear equations:

\[ f_i(x) \approx c_i, \quad i = 1, 2, \cdots, m. \]

The nonlinear least squares (NLS) problem is formulated as

\[
\min_{x \in \mathbb{R}^n} \sum_{i=1}^{m} (f_i(x) - c_i)^2.
\]

The Gauss-Newton method is specifically devised to solve NLS problems of the form, but the method is not guaranteed to converge to the global optimal solution but rather to a stationary point (see §4.5).
Circle fitting

Suppose that we are given $m$ points $a_1, a_2, \cdots, a_m \in \mathbb{R}^n$. The circle fitting problem seeks to find a circle with center $x$ and radius $r$

$$C(x, r) := \{y \in \mathbb{R}^n : \|y - x\| = r\},$$

that best fits the $m$ points. The nonlinear (approximate) equations associated with the problem are

$$\|x - a_i\| \approx r, \quad i = 1, 2, \cdots, m.$$

Since we wish to deal with differentiable functions, we will consider the squared version

$$\|x - a_i\|^2 \approx r^2, \quad i = 1, 2, \cdots, m.$$

The NLS problem associated with these equations is

$$\min_{x \in \mathbb{R}^n, r \geq 0} \sum_{i=1}^{m} (\|x - a_i\|^2 - r^2)^2$$
Equivalent to a linear LS problem

The above NLS problem is the same as

$$\min \left\{ \sum_{i=1}^{m} \left( -2a_i^\top x + \|x\|^2 - r^2 + \|a_i\|^2 \right)^2 : x \in \mathbb{R}^n, r \in \mathbb{R} \right\}.$$  

Making the change of variables $R := \|x\|^2 - r^2$, it reduces to

$$\min_{x \in \mathbb{R}^n, R \in \mathbb{R}} \left\{ f(x, R) := \sum_{i=1}^{m} \left( -2a_i^\top x + R + \|a_i\|^2 \right)^2 : \|x\|^2 \geq R \right\}.$$  

Indeed, any optimal solution $(\hat{x}, \hat{R})$ automatically satisfies $\|\hat{x}\|^2 \geq \hat{R}$, since otherwise, if $\|\hat{x}\|^2 < \hat{R}$, we would have for $i = 1, 2, \cdots, m$,

$$-2a_i^\top \hat{x} + \hat{R} + \|a_i\|^2 > -2a_i^\top \hat{x} + \|\hat{x}\|^2 + \|a_i\|^2 = \|\hat{x} - a_i\|^2 \geq 0.$$  

Squaring both sides and summing over $i$ yield

$$f(\hat{x}, \hat{R}) = \sum_{i=1}^{m} \left( -2a_i^\top \hat{x} + \hat{R} + \|a_i\|^2 \right)^2 > \sum_{i=1}^{m} \left( -2a_i^\top \hat{x} + \|\hat{x}\|^2 + \|a_i\|^2 \right)^2$$

$$= f(\hat{x}, \|\hat{x}\|^2).$$  

This is a contradiction, since $(\hat{x}, \hat{R})$ is an optimal solution.
Equivalent to a linear LS problem (cont’d)

Finally, we have the linear least squares problem:

\[
\min_{y \in \mathbb{R}^{n+1}} \| \tilde{A} y - b \|^2,
\]

where \( y = (x, R)^\top \) and

\[
\tilde{A} = \begin{bmatrix}
2a_1^\top & -1 \\
2a_2^\top & -1 \\
\vdots & \vdots \\
2a_m^\top & -1 
\end{bmatrix}, \quad b = \begin{bmatrix}
\|a_1\|^2 \\
\|a_2\|^2 \\
\vdots \\
\|a_m\|^2 
\end{bmatrix}.
\]

If \( \tilde{A} \) is of full column rank, then the unique solution is

\[
y = (\tilde{A}^\top \tilde{A})^{-1} \tilde{A}^\top b,
\]

and the radius \( r \) is given by \( r = \sqrt{\|x\|^2 - R} \).
Example: the best circle fitting of 10 points

The best circle fitting of 10 points denoted by asterisks.