Least Squares with Examples in Signal Processing*

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Abstract

These notes address the calculation and applications of approximate solutions to linear equations by least squares. Least squares is illustrated by way of several examples in signal processing: linear prediction, smoothing, deconvolution, system identification, and estimating missing data.

These notes address the calculation and applications of approximate solutions to linear equations by least squares. We deal with the 'easy' case wherein the system matrix is full rank. If the system matrix is rank deficient, then other methods are needed, e.g., QR decomposition, singular value decomposition, or the pseudo-inverse, [2], [3].

In these notes, least squares is illustrated by applying it to several basic problems in signal processing:

1. Linear prediction
2. Smoothing
3. Deconvolution
4. System identification
5. Estimating missing data

For the use of least squares in filter design, see [1].

1 Notation

We denote vectors in lower-case bold, i.e.,

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}. \tag{1}$$

We denote matrices in upper-case bold. The transpose of a vector or matrix in indicated by a superscript T, i.e., $\mathbf{x}^T$ is the transpose of $\mathbf{x}$.

*Version 1.1: Apr 17, 2013 10:08 pm +0000

The notation $\| \mathbf{x} \|_2$ refers to the Euclidian length of the vector $\mathbf{x}$, i.e.,

$$\| \mathbf{x} \|_2 = \sqrt{|x_1|^2 + |x_2|^2 + \cdots + |x_N|^2}. \tag{2}$$

The 'sum of squares' of $\mathbf{x}$ is denoted by $\| \mathbf{x} \|_2^2$, i.e.,

$$\| \mathbf{x} \|_2^2 = \sum_n |x(n)|^2 = \mathbf{x}^T \mathbf{x}. \tag{3}$$

The 'energy' of a vector $\mathbf{x}$ refers to $\| \mathbf{x} \|_2^2$.

In these notes, it is assumed that all vectors and matrices are real-valued. In the complex-valued case, the conjugate transpose should be used in place of the transpose, etc.

2 Overdetermined equations

Consider the system of linear equations

$$\mathbf{y} = \mathbf{H}\mathbf{x}. \tag{4}$$

If there is no solution to this system of equations, then the system is 'overdetermined'. This frequently happens when $\mathbf{H}$ is a 'tall' matrix (more rows than columns) with linearly independent columns.

In this case, it is common to seek a solution $\mathbf{x}$ minimizing the energy of the error:

$$J(\mathbf{x}) = \| \mathbf{y} - \mathbf{H}\mathbf{x} \|_2^2 . \tag{5}$$

Expanding $J(\mathbf{x})$ gives

$$\begin{aligned} J(\mathbf{x}) &= (\mathbf{y} - \mathbf{H}\mathbf{x})^T (\mathbf{y} - \mathbf{H}\mathbf{x}) \\ &= \mathbf{y}^T\mathbf{y} - \mathbf{y}^T\mathbf{H}\mathbf{x} - \mathbf{x}^T\mathbf{H}^T\mathbf{y} + \mathbf{x}^T\mathbf{H}^T\mathbf{H}\mathbf{x} \\ &= \mathbf{y}^T\mathbf{y} - 2\mathbf{y}^T\mathbf{H}\mathbf{x} + \mathbf{x}^T\mathbf{H}^T\mathbf{H}\mathbf{x}. \end{aligned} \tag{6}$$

Note that each of the four terms in (6) are scalars. Note also that the scalar $\mathbf{x}^T\mathbf{H}^T\mathbf{y}$ is the transpose of the scalar $\mathbf{y}^T\mathbf{H}\mathbf{x}$, and hence $\mathbf{x}^T\mathbf{H}^T\mathbf{y} = \mathbf{y}^T\mathbf{H}\mathbf{x}$.

Taking the derivative (see Appendix "Vector derivatives" (Section 10: Vector derivatives)), gives

$$\frac{\partial}{\partial \mathbf{x}} J(\mathbf{x}) = -2\mathbf{H}^T\mathbf{y} + 2\mathbf{H}^T\mathbf{H}\mathbf{x} \tag{7}$$

Setting the derivative to zero,

$$\frac{\partial}{\partial \mathbf{x}} J(\mathbf{x}) = \mathbf{0} \quad \Rightarrow \quad \mathbf{H}^T\mathbf{H}\mathbf{x} = \mathbf{H}^T\mathbf{y} \tag{8}$$

Let us assume that $\mathbf{H}^T\mathbf{H}$ is invertible. Then the solution is given by

$$\mathbf{x} = \left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{H}^T\mathbf{y}. \tag{9}$$

This is the 'least squares' solution.

$$\boxed{\min_{\mathbf{x}} \; \| \mathbf{y} - \mathbf{H}\mathbf{x} \|_2^2 \qquad \Rightarrow \qquad \mathbf{x} = \left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{H}^T\mathbf{y}} \tag{10}$$

In some situations, it is desirable to minimize the *weighted* square error, i.e., $\sum_n w_n r_n^2$ where $\mathbf{r}$ is the residual, or error, $\mathbf{r} = \mathbf{y} - \mathbf{H}\mathbf{x}$, and w_n are positive weights. This corresponds to minimizing $\| \mathbf{W}^{1/2} (\mathbf{y} - \mathbf{H}\mathbf{x}) \|_2^2$ where $\mathbf{W}$ is the diagonal matrix, $[\mathbf{W}]_{n,n} = w_n$. Using (10) gives

$$\min_{\mathbf{x}} \; \| \mathbf{W}^{1/2} (\mathbf{y} - \mathbf{H}\mathbf{x}) \|_2^2 \qquad \Rightarrow \qquad \mathbf{x} = \left(\mathbf{H}^T\mathbf{W}\mathbf{H}\right)^{-1}\mathbf{H}^T\mathbf{W}\mathbf{y} \tag{11}$$

where we have used the fact that $\mathbf{W}$ is symmetric.

3 Underdetermined equations

Consider the system of linear equations

$$\mathbf{y} = \mathbf{H}\mathbf{x}. \tag{12}$$

If there are many solutions, then the system is 'underdetermined'. This frequently happens when $\mathbf{H}$ is a 'wide' matrix (more columns than rows) with linearly independent rows.

In this case, it is common to seek a solution $\mathbf{x}$ with minimum norm. That is, we would like to solve the optimization problem

$$\begin{aligned} \underset{\mathbf{x}}{min} \quad & \| \mathbf{x} \|_2^2 \\ \text{such that} \quad & \mathbf{y} = \mathbf{H}\mathbf{x}. \end{aligned} \tag{13}$$

Minimization with constraints can be done with Lagrange multipliers. So, define the Lagrangian:

$$\mathcal{L}(\mathbf{x}, \mu) = \| \mathbf{x} \|_2^2 + \mu^T (\mathbf{y} - \mathbf{H}\mathbf{x}) \tag{14}$$

Take the derivatives of the Lagrangian:

$$\begin{aligned} \tfrac{\partial}{\partial \mathbf{x}} \mathcal{L}(\mathbf{x}) &= 2\mathbf{x} - \mathbf{H}^T \mu \\ \tfrac{\partial}{\partial \mu} \mathcal{L}(\mathbf{x}) &= \mathbf{y} - \mathbf{H}\mathbf{x} \end{aligned} \tag{15}$$

Set the derivatives to zero to get:

$$\begin{aligned} \mathbf{x} &= \tfrac{1}{2} \mathbf{H}^T \mu \\ \mathbf{y} &= \mathbf{H}\mathbf{x} \end{aligned} \tag{16}$$

Plugging (16) into gives

$$\mathbf{y} = \frac{1}{2} \mathbf{H}\mathbf{H}^T \mu. \tag{17}$$

Let us assume $\mathbf{H}\mathbf{H}^T$ is invertible. Then

$$\mu = 2\left(\mathbf{H}\mathbf{H}^T\right)^{-1} \mathbf{y}. \tag{18}$$

Plugging (18) into (16) gives the 'least squares' solution:

$$\mathbf{x} = \mathbf{H}^T \left(\mathbf{H}\mathbf{H}^T\right)^{-1} \mathbf{y}. \tag{19}$$

We can verify that $\mathbf{x}$ in this formula does in fact satisfy $\mathbf{y} = \mathbf{H}\mathbf{x}$ by plugging in:

$$\mathbf{H}\mathbf{x} = \mathbf{H}\left[\mathbf{H}^T \left(\mathbf{H}\mathbf{H}^T\right)^{-1} \mathbf{y}\right] = \left(\mathbf{H}\mathbf{H}^T\right) \left(\mathbf{H}\mathbf{H}^T\right)^{-1} \mathbf{y} = \mathbf{y} \tag{20}$$

So,

$$\boxed{\underset{\mathbf{x}}{min} \ \| \mathbf{x} \|_2^2 \quad \text{s.t.} \quad \mathbf{y} = \mathbf{H}\mathbf{x} \qquad \Rightarrow \qquad \mathbf{x} = \mathbf{H}^T \left(\mathbf{H}\mathbf{H}^T\right)^{-1} \mathbf{y}.} \tag{21}$$

In some situations, it is desirable to minimize the *weighted* energy, i.e., $\sum_n w_n \, x_n^2$, where w_n are positive weights. This corresponds to minimizing $\| \mathbf{W}^{1/2} \, \mathbf{x} \|_2^2$ where $\mathbf{W}$ is the diagonal matrix, $[\mathbf{W}]_{n,n} = w_n$. The derivation of the solution is similar, and gives

$$\underset{\mathbf{x}}{min} \ \ \| \mathbf{W}^{1/2}\mathbf{x} \|_2^2 \quad \text{s.t. } \mathbf{y} = \mathbf{H}\mathbf{x} \quad \Rightarrow \quad \mathbf{x} = \mathbf{W}^{-1} \, \mathbf{H}^T \left(\mathbf{H}\mathbf{W}^{-1}\mathbf{H}^T \right)^{-1} \mathbf{y} \tag{22}$$

This solution is also derived below, see (45).

4 Regularization

In the overdetermined case, we minimized $\| \mathbf{y} - \mathbf{H}\mathbf{x} \|_2^2$. In the underdetermined case, we minimized $\| \mathbf{x} \|_2^2$. Another approach is to minimize the weighted sum: $c_1 \ \| \mathbf{y} - \mathbf{H}\mathbf{x} \|_2^2 + c_2 \ \| \mathbf{x} \|_2^2$. The solution $\mathbf{x}$ depends on the ratio c_2/c_1, not on c_1 and c_2 individually.

A common approach to obtain an inexact solution to a linear system is to minimize the objective function:

$$J(\mathbf{x}) = \| \mathbf{y} - \mathbf{H}\mathbf{x} \|_2^2 + \lambda \ \| \mathbf{x} \|_2^2 \tag{23}$$

where $\lambda > 0$. Taking the derivative, we get

$$\frac{\partial}{\partial \mathbf{x}} J(\mathbf{x}) = 2\mathbf{H}^T (\mathbf{H}\mathbf{x} - \mathbf{y}) + 2\lambda \mathbf{x} \tag{24}$$

Setting the derivative to zero,

$$\begin{aligned} \tfrac{\partial}{\partial \mathbf{x}} J(\mathbf{x}) = \mathbf{0} \qquad & \Rightarrow \quad \mathbf{H}^T\mathbf{H}\mathbf{x} + \lambda\mathbf{x} = \mathbf{H}^T\mathbf{y} \\ & \Rightarrow \quad \left(\mathbf{H}^T\mathbf{H} + \lambda\mathbf{I} \right) \mathbf{x} = \mathbf{H}^T\mathbf{y} \end{aligned} \tag{25}$$

So the solution is given by

$$\mathbf{x} = \left(\mathbf{H}^T\mathbf{H} + \lambda\mathbf{I} \right)^{-1} \mathbf{H}^T\mathbf{y} \tag{26}$$

So,

$$\boxed{\underset{\mathbf{x}}{min} \ \ \| \mathbf{y} - \mathbf{H}\mathbf{x} \|_2^2 + \lambda \ \| \mathbf{x} \|_2^2 \quad \Rightarrow \quad \mathbf{x} = \left(\mathbf{H}^T\mathbf{H} + \lambda\mathbf{I} \right)^{-1} \mathbf{H}^T\mathbf{y}} \tag{27}$$

This is referred to as 'diagonal loading' because a constant, λ, is added to the diagonal elements of $\mathbf{H}^T\mathbf{H}$. The approach also avoids the problem of rank deficiency because $\mathbf{H}^T\mathbf{H} + \lambda\mathbf{I}$ is invertible even if $\mathbf{H}^T\mathbf{H}$ is not. In addition, the solution (27) can be used in both cases: when $\mathbf{H}$ is tall and when $\mathbf{H}$ is wide.

5 Weighted regularization

A more general form of the regularized objective function (23) is:

$$J(\mathbf{x}) = \| \mathbf{y} - \mathbf{H}\mathbf{x} \|_2^2 + \lambda \ \| \mathbf{A}\mathbf{x} \|_2^2 \tag{28}$$

where $\lambda > 0$. Taking the derivative, we get

$$\frac{\partial}{\partial \mathbf{x}} J(\mathbf{x}) = 2\mathbf{H}^T (\mathbf{H}\mathbf{x} - \mathbf{y}) + 2\lambda \mathbf{A}^T\mathbf{A}\mathbf{x} \tag{29}$$

Setting the derivative to zero,

$$\begin{aligned} \tfrac{\partial}{\partial \mathbf{x}} J(\mathbf{x}) = \mathbf{0} \qquad & \Rightarrow \quad \mathbf{H}^T\mathbf{H}\mathbf{x} + \lambda\mathbf{A}^T\mathbf{A}\mathbf{x} = \mathbf{H}^T\mathbf{y} \\ & \Rightarrow \quad \left(\mathbf{H}^T\mathbf{H} + \lambda\mathbf{A}^T\mathbf{A} \right) \mathbf{x} = \mathbf{H}^T\mathbf{y} \end{aligned} \tag{30}$$

So the solution is given by

$$\mathbf{x} = \left(\mathbf{H}^T\mathbf{H} + \lambda\mathbf{A}^T\mathbf{A}\right)^{-1}\mathbf{H}^T\mathbf{y} \tag{31}$$

So,

$$\boxed{\begin{array}{c} \underset{\mathbf{x}}{min} \;\; \| \mathbf{y} - \mathbf{H}\mathbf{x} \|_2^2 + \lambda \; \| \mathbf{A}\mathbf{x} \|_2^2 \\ \Rightarrow \quad \mathbf{x} = \left(\mathbf{H}^T\mathbf{H} + \lambda\mathbf{A}^T\mathbf{A}\right)^{-1}\mathbf{H}^T\mathbf{y} \end{array}} \tag{32}$$

Note that if $\mathbf{A}$ is the identity matrix, then equation (32) becomes (27).

6 Constrained least squares

Constrained least squares refers to the problem of finding a least squares solution that exactly satisfies additional constraints. If the additional constraints are a set of linear equations, then the solution is obtained as follows.

The constrained least squares problem is of the form:

$$\begin{array}{c} \underset{\mathbf{x}}{min} \;\; \| \mathbf{y} - \mathbf{H}\mathbf{x} \|_2^2 \\ \text{such that } \mathbf{C}\mathbf{x} = \mathbf{b} \end{array} \tag{33}$$

Define the Lagrangian,

$$\mathcal{L}\left(\mathbf{x}, \mu\right) = \| \mathbf{y} - \mathbf{H}\mathbf{x} \|_2^2 + \mu^T\left(\mathbf{C}\mathbf{x} - \mathbf{b}\right). \tag{34}$$

The derivatives are:

$$\frac{\partial}{\partial \mathbf{x}}\mathcal{L}\left(\mathbf{x}\right) = 2\mathbf{H}^T\left(\mathbf{H}\mathbf{x} - \mathbf{y}\right) + \mathbf{C}^T\mu \tag{35}$$

$$\frac{\partial}{\partial \mu}\mathcal{L}\left(\mathbf{x}\right) = \mathbf{C}\mathbf{x} - \mathbf{b} \tag{36}$$

Setting the derivatives to zero,

$$\begin{array}{c} \frac{\partial}{\partial \mathbf{x}}\mathcal{L}\left(\mathbf{x}\right) = \mathbf{0} \quad \Rightarrow \quad \mathbf{x} = \left(\mathbf{H}^T\mathbf{H}\right)^{-1}\left(\mathbf{H}^T\mathbf{y} - 0.5\mathbf{C}^T\mu\right) \\ \frac{\partial}{\partial \mu}\mathcal{L}\left(\mathbf{x}\right) = \mathbf{0} \quad \Rightarrow \quad \mathbf{C}\mathbf{x} = \mathbf{b} \end{array} \tag{37}$$

Multiplying (37) on the left by $\mathbf{C}$ gives $\mathbf{C}\mathbf{x}$, which from is $\mathbf{b}$, so we have

$$\mathbf{C}\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\left(\mathbf{H}^T\mathbf{y} - 0.5\mathbf{C}^T\mu\right) = \mathbf{b} \tag{38}$$

or, expanding,

$$\mathbf{C}\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{H}^T\mathbf{y} - 0.5\mathbf{C}\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{C}^T\mu = \mathbf{b}. \tag{39}$$

Solving for μ gives

$$\mu = 2\left(\mathbf{C}\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{C}^T\right)^{-1}\left(\mathbf{C}\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{H}^T\mathbf{y} - \mathbf{b}\right) \tag{40}$$

Plugging μ into (37) gives

$$\mathbf{x} = \left(\mathbf{H}^T\mathbf{H}\right)^{-1}\left(\mathbf{H}^T\mathbf{y} - \mathbf{C}^T\left(\mathbf{C}\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{C}^T\right)^{-1}\left(\mathbf{C}\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{H}^T\mathbf{y} - \mathbf{b}\right)\right) \tag{41}$$

Let us verify that $\mathbf{x}$ in this formula does in fact satisfy $\mathbf{Cx} = \mathbf{b}$,

$$\begin{aligned}\mathbf{Cx} &= \mathbf{C}\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\left(\mathbf{H}^T\mathbf{y} - \mathbf{C}^T\left(\mathbf{C}\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{C}^T\right)^{-1}\left(\mathbf{C}\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{H}^T\mathbf{y} - \mathbf{b}\right)\right) \\ &= \mathbf{C}\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{H}^T\mathbf{y} - \mathbf{C}\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{C}^T\left(\mathbf{C}\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{C}^T\right)^{-1}\left(\mathbf{C}\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{H}^T\mathbf{y} - \mathbf{b}\right) \\ &= \mathbf{C}\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{H}^T\mathbf{y} - \left(\mathbf{C}\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{H}^T\mathbf{y} - \mathbf{b}\right) \\ &= \mathbf{b}\end{aligned} \tag{42}$$

So,

$$\boxed{\begin{array}{c}\underset{\mathbf{x}}{min} \ \parallel \mathbf{y} - \mathbf{Hx} \parallel_2^2 \quad \text{s.t.} \quad \mathbf{Cx} = \mathbf{b} \quad \Rightarrow \\ \mathbf{x} = \left(\mathbf{H}^T\mathbf{H}\right)^{-1}\left(\mathbf{H}^T\mathbf{y} - \mathbf{C}^T\left(\mathbf{C}\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{C}^T\right)^{-1}\left(\mathbf{C}\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{H}^T\mathbf{y} - \mathbf{b}\right)\right)\end{array}} \tag{43}$$

6.1 Special cases

Simpler forms of (43) are frequently useful. For example, if $\mathbf{H} = \mathbf{I}$ and $\mathbf{b} = \mathbf{0}$ in (43), then we get

$$\boxed{\begin{array}{c}\underset{\mathbf{x}}{min} \ \parallel \mathbf{y} - \mathbf{x} \parallel_2^2 \quad \text{s.t.} \quad \mathbf{Cx} = \mathbf{0} \\ \Rightarrow \quad \mathbf{x} = \mathbf{y} - \mathbf{C}^T\left(\mathbf{CC}^T\right)^{-1}\mathbf{Cy}\end{array}} \tag{44}$$

If $\mathbf{y} = \mathbf{0}$ in (43), then we get

$$\boxed{\begin{array}{c}\underset{\mathbf{x}}{min} \ \parallel \mathbf{Hx} \parallel_2^2 \quad \text{s.t.} \quad \mathbf{Cx} = \mathbf{b} \\ \Rightarrow \quad \mathbf{x} = \left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{C}^T\left(\mathbf{C}\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{C}^T\right)^{-1}\mathbf{b}\end{array}} \tag{45}$$

If $\mathbf{y} = \mathbf{0}$ and $\mathbf{H} = \mathbf{I}$ in (43), then we get

$$\boxed{\underset{\mathbf{x}}{min} \ \parallel \mathbf{x} \parallel_2^2 \quad \text{s.t.} \quad \mathbf{Cx} = \mathbf{b} \quad \Rightarrow \quad \mathbf{x} = \mathbf{C}^T\left(\mathbf{CC}^T\right)^{-1}\mathbf{b}} \tag{46}$$

which is the same as (21).

7 Note

The expressions above involve matrix inverses. For example, (10) involves $\left(\mathbf{H}^T\mathbf{H}\right)^{-1}$. However, it must be emphasized that finding the least square solution does not require computing the inverse of $\mathbf{H}^T\mathbf{H}$ even though the inverse appears in the formula. Instead, $\mathbf{x}$ in (10) should be obtained, in practice, by solving the system $\mathbf{Ax} = \mathbf{b}$ where $\mathbf{A} = \mathbf{H}^T\mathbf{H}$ and $\mathbf{b} = \mathbf{H}^T\mathbf{y}$. The most direct way to solve a linear system of equations is by Gaussian elimination. Gaussian elimination is much faster than computing the inverse of the matrix $\mathbf{A}$.

8 Examples

8.1 Polynomial approximation

An important example of least squares is fitting a low-order polynomial to data. Suppose the N-point data is of the form $(t_i,\, y_i)$ for $1 \le i \le N$.

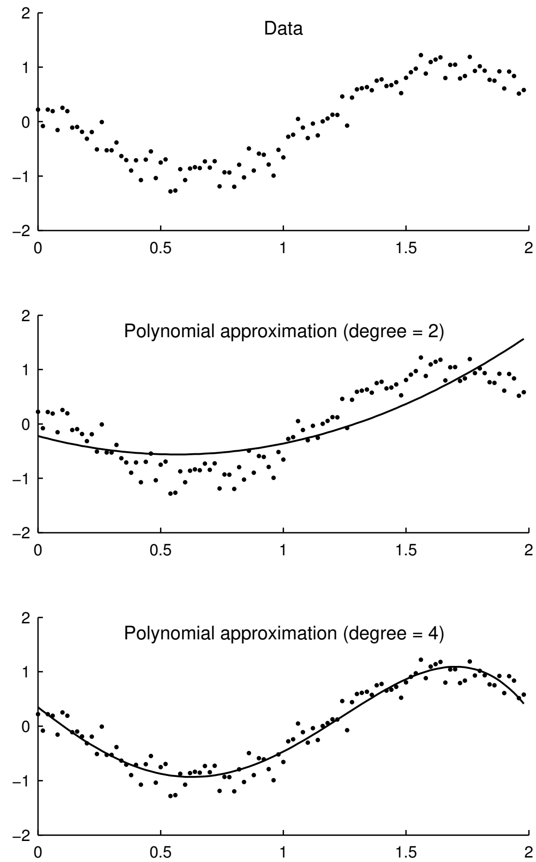


Figure 46: Least squares polynomial approximation.

The goal is to find a polynomial that approximates the data by minimizing the energy of the residual:

$$E = \sum_i \left(y_i - p\left(t_i\right)\right)^2 \tag{47}$$

where $p\left(t\right)$ is a polynomial, e.g.,

$$p\left(t\right) = a_0 + a_1\, t + a_2\, t^2. \tag{48}$$

The problem can be viewed as solving the overdetermined system of equations,

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \approx \begin{bmatrix} 1 & t_1 & t_1^2 \\ 1 & t_2 & t_2^2 \\ \vdots & \vdots & \vdots \\ 1 & t_N & t_N^2 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix}, \tag{49}$$

which we denote as $\mathbf{y} \approx \mathbf{Ha}$. The energy of the residual, E, is written as

$$E = \| \mathbf{y} - \mathbf{Ha} \|_2^2 . \tag{50}$$

From (10), the least squares solution is given by $\mathbf{a} = \left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{H}^T\mathbf{y}$. An example is illustrated in Figure 46.

8.2 Linear prediction

One approach to predict future values of a time-series is based on linear prediction, e.g.,

$$y(n) \approx a_1\, y(n-1) + a_2\, y(n-2) + a_3\, y(n-3) . \tag{51}$$

If past data $y(n)$ is available, then the problem of finding a_i can be solved using least squares. Finding $\mathbf{a} = (a_0,\, a_1,\, a_2)^T$ can be viewed as one of solving an overdetermined system of equations. For example, if $y(n)$ is available for $0 \le n \le N-1$, and we seek a third order linear predictor, then the overdetermined system of equations are given by

$$\begin{bmatrix} y(3) \\ y(4) \\ \vdots \\ y(N-1) \end{bmatrix} \approx \begin{bmatrix} y(2) & y(1) & y(0) \\ y(3) & y(2) & y(1) \\ \vdots & \vdots & \vdots \\ y(N-2) & y(N-3) & y(N-4) \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}, \tag{52}$$

which we can write as $\overline{\mathbf{y}} = \mathbf{Ha}$ where $\mathbf{H}$ is a matrix of size $(N-3) \times 3$. From (10), the least squares solution is given by $\mathbf{a} = \left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{H}^T\overline{\mathbf{y}}$. Note that $\mathbf{H}^T\mathbf{H}$ is small, of size 3×3 only. Hence, $\mathbf{a}$ is obtained by solving a small linear system of equations.

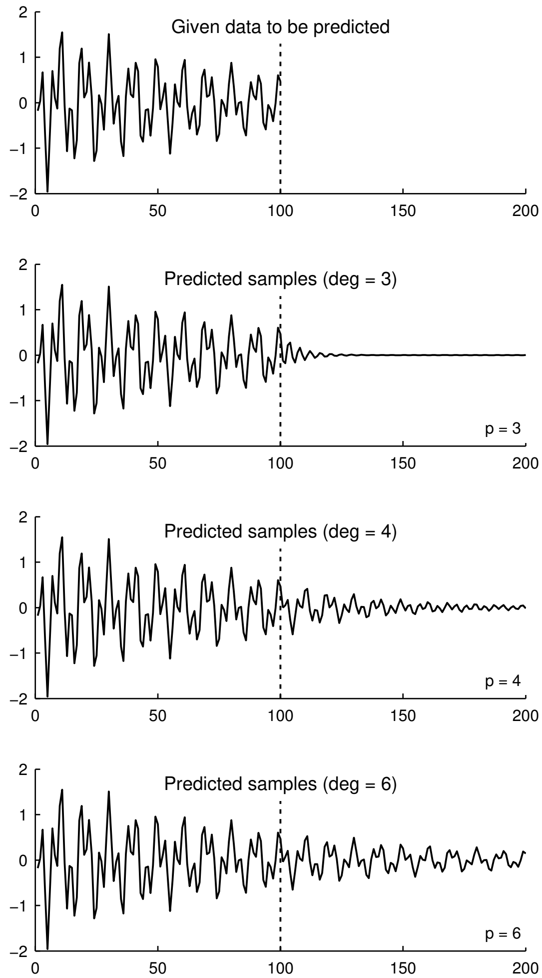


Figure 52: Least squares linear prediction.

Once the coefficients a_i are found, then $y(n)$ for $n > N$ can be estimated using the recursive difference equation (51).

An example is illustrated in Figure 52. One hundred samples of data are available, i.e., $y(n)$ for $0 \le n \le 99$. From these 100 samples, a p-order linear predictor is obtained by least squares, and the subsequent 100 samples are predicted.

8.3 Smoothing

One approach to smooth a noisy signal is based on least squares weighted regularization. The idea is to obtain a signal similar to the noisy one, but smoother. The smoothness of a signal can be measured by the energy of its derivative (or second-order derivative). The smoother a signal is, the smaller the energy of its derivative is.

Define the matrix $\mathbf{D}$ as

$$\mathbf{D} = \begin{bmatrix} 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & & \ddots & \\ & & & 1 & -2 & 1 \end{bmatrix}. \quad (53)$$

Then $\mathbf{Dx}$ is the second-order difference (a discrete form of the second-order derivative) of the signal $x(n)$. See Appendix "The Kth-order difference" (Section 11: The Kth-order difference). If $\mathbf{x}$ is smooth, then $\| \mathbf{Dx} \|_2^2$ is small in value.

If $y(n)$ is a noisy signal, then a smooth signal $x(n)$, that approximates $y(n)$, can be obtained as the solution to the problem:

$$\underset{\mathbf{x}}{min} \ \| \mathbf{y} - \mathbf{x} \|_2^2 + \lambda \| \mathbf{Dx} \|_2^2 \quad (54)$$

where $\lambda > 0$ is a parameter to be specified. Minimizing $\| \mathbf{y} - \mathbf{x} \|_2^2$ forces $\mathbf{x}$ to be similar to the noisy signal $\mathbf{y}$. Minimizing $\| \mathbf{Dx} \|_2^2$ forces $\mathbf{x}$ to be smooth. Minimizing the sum in (54) forces $\mathbf{x}$ to be both similar to $\mathbf{y}$ and smooth (as far as possible, and depending on λ).

If $\lambda = 0$, then the solution will be the noisy data, i.e., $\mathbf{x} = \mathbf{y}$, because this solution makes (54) equal to zero. In this case, no smoothing is achieved. On the other hand, the greater λ is, the smoother $\mathbf{x}$ will be.

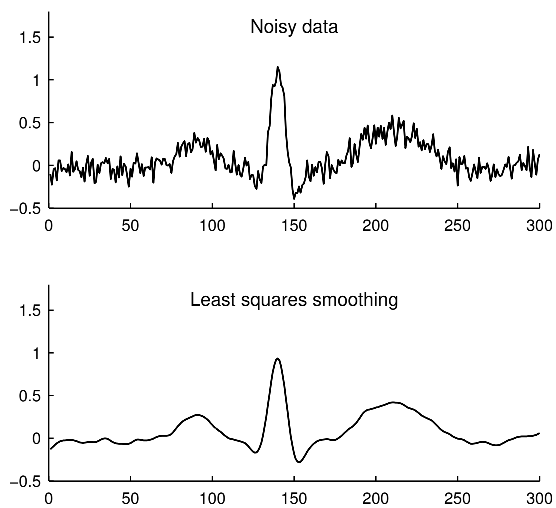


Figure 54: Least squares smoothing.

Using (32), the signal $\mathbf{x}$ minimizing (54) is given by

$$\mathbf{x} = \left(\mathbf{I} + \lambda \mathbf{D}^T \mathbf{D}\right)^{-1} \mathbf{y}. \quad (55)$$

Note that the matrix $\mathbf{I} + \lambda \mathbf{D}^T \mathbf{D}$ is banded. (The only non-zero values are near the main diagonal). Therefore, the solution can be obtained using fast solvers for banded systems [5].

An example of least squares smoothing is illustrated in Figure 54. A noisy ECG signal is smoothed using (55). We have used the ECG waveform generator ECGSYN [4].

8.4 Deconvolution

Deconvolution refers to the problem of finding the input to an LTI system when the output signal is known. Here, we assume the impulse response of the system is known. The output, $y(n)$, is given by

$$y(n) = h(0)\, x(n) + h(1)\, x(n-1) + \cdots + h(N)\, x(n-N) \tag{56}$$

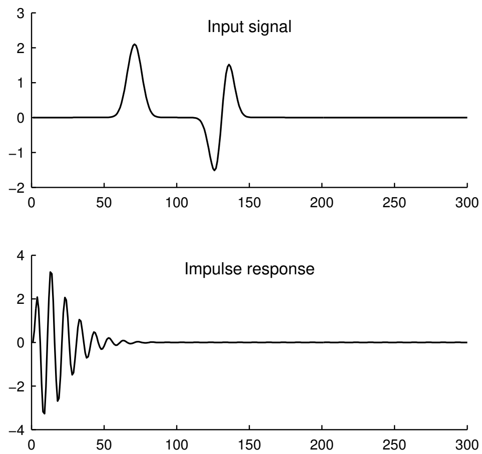
where $x(n)$ is the input signal and $h(n)$ is the impulse response. Equation (56) can be written as $\mathbf{y} = \mathbf{H}\mathbf{x}$ where $\mathbf{H}$ is a matrix of the form

$$\mathbf{H} = \begin{bmatrix} h(0) & & & \\ h(1) & h(0) & & \\ h(2) & h(1) & h(0) & \\ \vdots & & & \ddots \end{bmatrix}. \tag{57}$$

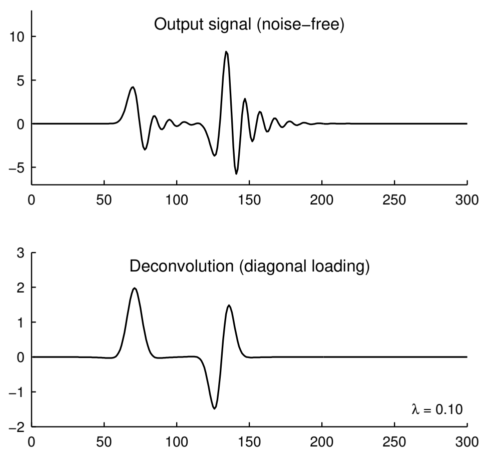
This matrix is constant-valued along its diagonals. Such matrices are called Toeplitz matrices.

It may be expected that $\mathbf{x}$ can be obtained from $\mathbf{y}$ by solving the linear system $\mathbf{y} = \mathbf{H}\mathbf{x}$. In some situations, this is possible. However, the matrix $\mathbf{H}$ is often singular or almost singular. In this case, Gaussian elimination encounters division by zeros.

For example, Figure 57 illustrates an input signal, $x(n)$, an impulse response, $h(n)$, and the output signal, $y(n)$. When we attempt to obtain $\mathbf{x}$ by solving $\mathbf{y} = \mathbf{H}\mathbf{x}$ in Matlab, we receive the warning message: `'Matrix is singular to working precision'` and we obtain a vector of all `NaN` (not a number).



(a)



(b)

Figure 57: Deconvolution of noise-free data by diagonal loading.

Due to $\mathbf{H}$ being singular, we regularize the problem. Note that the input signal is largely zero, hence, it is reasonable to seek a solution $\mathbf{x}$ with small energy. The signal $\mathbf{x}$ we seek should also satisfy $\mathbf{y} = \mathbf{H}\mathbf{x}$, at least approximately. To obtain such a signal, $\mathbf{x}$, we solve the problem:

$$\underset{\mathbf{x}}{min} \ \parallel \mathbf{y} - \mathbf{H}\mathbf{x} \parallel_2^2 + \lambda \parallel \mathbf{x} \parallel_2^2 \tag{58}$$

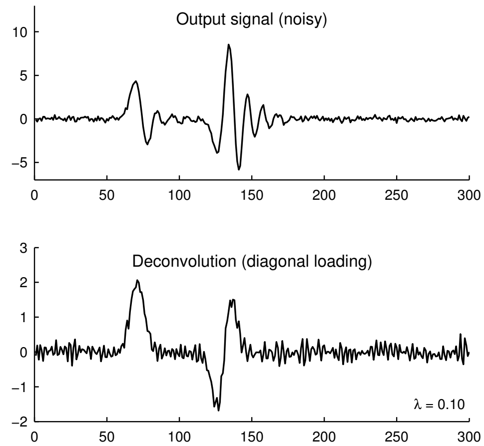
where $\lambda > 0$ is a parameter to be specified. Minimizing $\parallel \mathbf{y} - \mathbf{H}\mathbf{x} \parallel_2^2$ forces $\mathbf{x}$ to be consistent with the output signal $\mathbf{y}$. Minimizing $\parallel \mathbf{x} \parallel_2^2$ forces $\mathbf{x}$ to have low energy. Minimizing the sum in (58) forces $\mathbf{x}$ to be consistent with $\mathbf{y}$ and to have low energy (as far as possible, and depending on λ). Using (32), the signal $\mathbf{x}$

minimizing (58) is given by

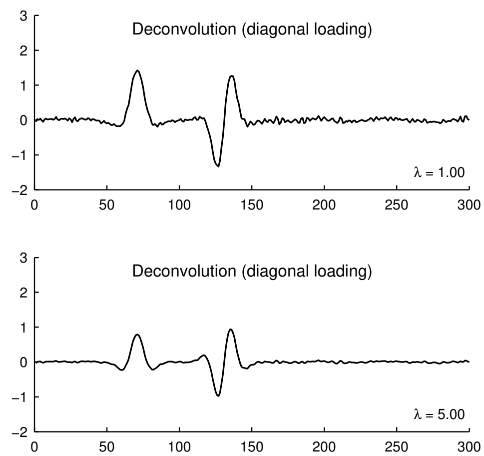
$$\mathbf{x} = \left(\mathbf{H}^T\mathbf{H} + \lambda\mathbf{I}\right)^{-1}\mathbf{H}^T\mathbf{y}. \tag{59}$$

This technique is called 'diagonal loading' because λ is added the diagonal of $\mathbf{H}^T\mathbf{H}$. A small value of λ is sufficient to make the matrix invertible. The solution, illustrated in Figure 57, is very similar to the original input signal, shown in the figure.

In practice, the available data is also noisy. In this case, the data $\mathbf{y}$ is given by $\mathbf{y} = \mathbf{H}\mathbf{x} + \mathbf{w}$ where $\mathbf{w}$ is the noise. The noise is often modeled as an additive white Gaussian random signal. In this case, diagonal loading with a small λ will generally produce a noisy estimate of the input signal. In Figure 57, we used $\lambda = 0.1$. When the same value is used with the noisy data, a noisy result is obtained, as illustrated in Figure 59. A larger λ is needed so as to attenuate the noise. But if λ is too large, then the estimate of the input signal is distorted. Notice that with $\lambda = 1.0$, the noise is reduced but the height of the the pulses present in the original signal are somewhat attenuated. With $\lambda = 5.0$, the noise is reduced slightly more, but the pulses are substantially more attenuated.



(a)



(b)

Figure 59: Deconvolution of noisy data by diagonal loading.

To improve the deconvolution result in the presence of noise, we can minimize the energy of the derivative (or second-order derivative) of $\mathbf{x}$ instead. As in the smoothing example above, minimizing the energy of the second-order derivative forces $\mathbf{x}$ to be smooth. In order that $\mathbf{x}$ is consistent with the data $\mathbf{y}$ and is also smooth, we solve the problem:

$$\underset{\mathbf{x}}{min} \ \parallel \mathbf{y} - \mathbf{H}\mathbf{x} \parallel_2^2 + \lambda \parallel \mathbf{D}\mathbf{x} \parallel_2^2 \tag{60}$$

where $\mathbf{D}$ is the second-order difference matrix (53). Using (32), the signal $\mathbf{x}$ minimizing (60) is given by

$$\mathbf{x} = \left(\mathbf{H}^T\mathbf{H} + \lambda\mathbf{D}^T\mathbf{D}\right)^{-1}\mathbf{H}^T\mathbf{y}. \tag{61}$$

The solution obtained using (61) is illustrated in Figure 61. Compared to the solutions obtained by diagonal loading, illustrated in Figure 59, this solution is less noisy and less distorted.

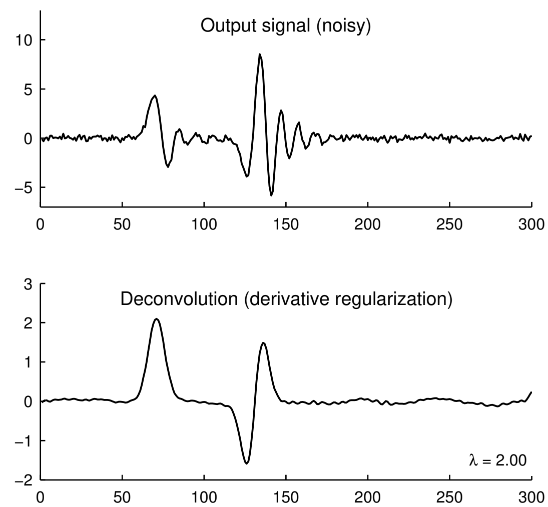
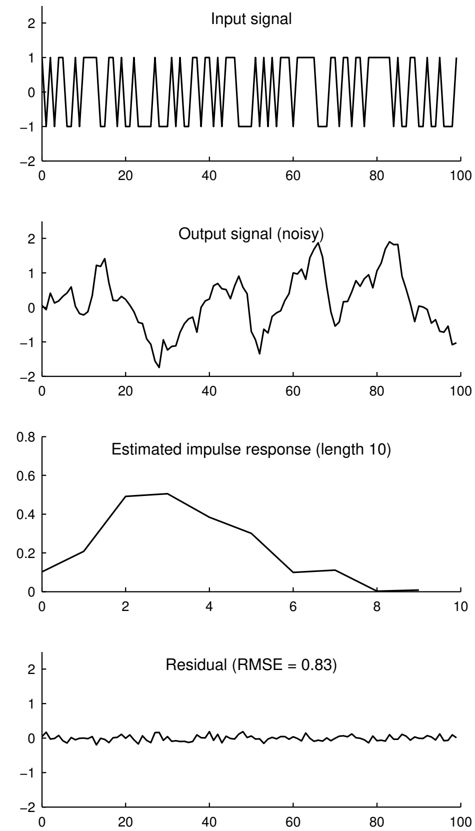


Figure 61: Deconvolution of noisy data by derivative regularization.

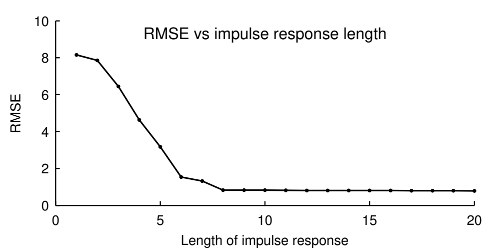
This example illustrates the need for regularization even when the data is noise-free (an unrealistic ideal case). It also illustrates the choice of regularizer (i.e., $\| \mathbf{x} \|_2^2$, $\| \mathbf{Dx} \|_2^2$, or other) affects the quality of the result.

8.5 System identification

System identification refers to the problem of estimating an unknown system. In its simplest form, the system is LTI and input-output data is available. Here, we assume that the output signal is noisy. We also assume that the impulse response is relatively short.



(a)



(b)

Figure 61: Least squares system identification.

The output, $y(n)$, of the system can be written as

$$y(n) = h_0\, x(n) + h_1\, x(n-1) + h_2\, x(n-2) + w(n) \tag{62}$$

where $x(n)$ is the input signal and $w(n)$ is the noise. Here, we have assumed the impulse response h_n is of length 3. We can write this in matrix form as

$$\begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \\ \vdots \end{bmatrix} \approx \begin{bmatrix} x_0 & & \\ x_1 & x_0 & \\ x_2 & x_1 & x_0 \\ x_3 & x_2 & x_1 \\ \vdots & & \vdots \end{bmatrix} \begin{bmatrix} h_0 \\ h_1 \\ h_2 \end{bmatrix} \tag{63}$$

which we denote as $\mathbf{y} \approx \mathbf{X}\mathbf{h}$. If $\mathbf{y}$ is much longer than the length of the impulse response $\mathbf{h}$, then $\mathbf{X}$ is a tall matrix and $\mathbf{y} \approx \mathbf{X}\mathbf{h}$ is an overdetermined system of equations. In this case, $\mathbf{h}$ can be estimated from (10) as

$$\mathbf{h} = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y} \tag{64}$$

An example is illustrated in Figure 61. A binary input signal and noisy output signal are shown. When it is assumed that $\mathbf{h}$ is of length 10, then we obtain the impulse response shown. The residual, i.e., $\mathbf{r} = \mathbf{y} - \mathbf{X}\mathbf{h}$, is also shown in the figure. It is informative to plot the root-mean-square-error (RMSE), i.e., $\parallel \mathbf{r} \parallel_2$, as a function of the length of the impulse response. This is a decreasing function. If the data really is the input-output data of an LTI system with a finite impulse response, and if the noise is not too severe, then the RMSE tends to flatten out at the correct impulse response length. This provides an indication of the length of the unknown impulse response.

8.6 Missing sample estimation

Due to transmission errors, transient interference, or impulsive noise, some samples of a signal may be lost or so badly corrupted as to be unusable. In this case, the missing samples should be estimated based on the available uncorrupted data. To complicate the problem, the missing samples may be randomly distributed through out the signal. Filling in missing values in order to conceal errors is called *error concealment*[6].

This example shows how the missing samples can be estimated by least squares. As an example, Figure 64 shows a 200-point ECG signal wherein 100 samples are missing. The problem is to fill in the missing 100 samples.

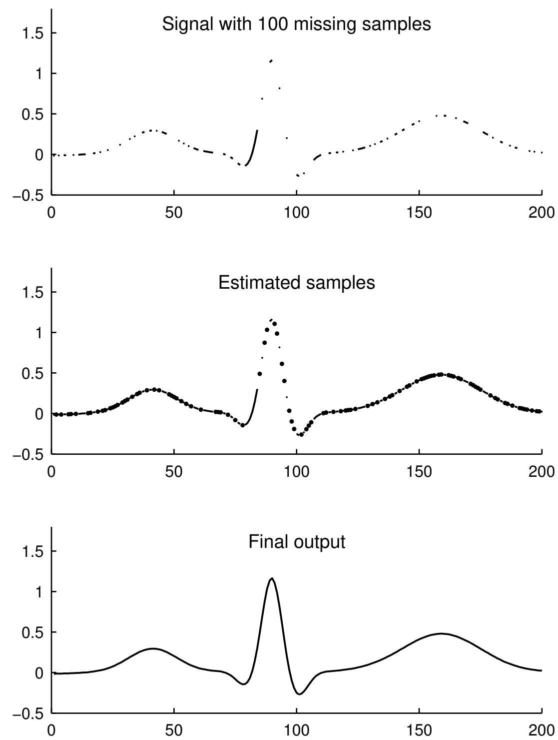


Figure 64: Least squares estimation of missing data.

To formulate the problem as a least squares problem, we introduce some notation. Let $\mathbf{x}$ be a signal of length N. Suppose K samples of $\mathbf{x}$ are known, where $K < N$. The K-point known signal, $\mathbf{y}$, can be written as

$$\mathbf{y} = \mathbf{S}\mathbf{x} \tag{65}$$

where $\mathbf{S}$ is a 'selection' (or 'sampling') matrix of size $K \times N$. For example, if only the first, second and last elements of a 5-point signal $\mathbf{x}$ are observed, then the matrix $\mathbf{S}$ is given by

$$\mathbf{S} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}. \tag{66}$$

The matrix $\mathbf{S}$ is the identity matrix with rows removed, corresponding to the missing samples. Note that

$\mathbf{Sx}$ removes two samples from the signal $\mathbf{x}$,

$$\mathbf{Sx} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x(0) \\ x(1) \\ x(2) \\ x(3) \\ x(4) \end{bmatrix} = \begin{bmatrix} x(0) \\ x(1) \\ x(4) \end{bmatrix} = \mathbf{y}. \tag{67}$$

The vector $\mathbf{y}$ consists of the *known* samples of $\mathbf{x}$. So, the vector $\mathbf{y}$ is shorter than $\mathbf{x}$ $(K < N)$.

The problem can be stated as: Given the signal, $\mathbf{y}$, and the matrix, $\mathbf{S}$, find $\mathbf{x}$ such that $\mathbf{y} = \mathbf{Sx}$. Of course, there are infinitely many solutions. Below, it is shown how to obtain a smooth solution by least squares.

Note that $\mathbf{S}^T\mathbf{y}$ has the effect of setting the missing samples to zero. For example, with $\mathbf{S}$ in (66) we have

$$\mathbf{S}^T\mathbf{y} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} y(0) \\ y(1) \\ y(2) \end{bmatrix} = \begin{bmatrix} y(0) \\ y(1) \\ 0 \\ 0 \\ y(2) \end{bmatrix}. \tag{68}$$

Let us define $\mathbf{S}_c$ as the 'complement' of $\mathbf{S}$. The matrix $\mathbf{S}_c$ consists of the rows of the identity matrix not appearing in $\mathbf{S}$. Continuing the 5-point example,

$$\mathbf{S}_c = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}. \tag{69}$$

Now, an estimate $\hat{\mathbf{x}}$ can be represented as

$$\hat{\mathbf{x}} = \mathbf{S}^T\mathbf{y} + \mathbf{S}_c^T\mathbf{v} \tag{70}$$

where $\mathbf{y}$ is the available data and $\mathbf{v}$ consists of the samples to be determined. For example,

$$\mathbf{S}^T\mathbf{y} + \mathbf{S}_c^T\mathbf{v} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} y(0) \\ y(1) \\ y(2) \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} v(0) \\ v(1) \end{bmatrix} = \begin{bmatrix} y(0) \\ y(1) \\ v(0) \\ v(1) \\ y(2) \end{bmatrix}. \tag{71}$$

The problem is to estimate the vector $\mathbf{v}$, which is of length $N - K$.

Let us assume that the original signal, $\mathbf{x}$, is smooth. Then it is reasonable to find $\mathbf{v}$ to optimize the smoothness of $\hat{\mathbf{x}}$, i.e., to minimize the energy of the second-order derivative of $\hat{\mathbf{x}}$. Therefore, $\mathbf{v}$ can be obtained by minimizing $\| \mathbf{D}\hat{\mathbf{x}} \|_2^2$ where $\mathbf{D}$ is the second-order difference matrix (53). Using (70), we find $\mathbf{v}$ by solving the problem

$$\min_{\mathbf{v}} \ \| \mathbf{D}\left(\mathbf{S}^T\mathbf{y} + \mathbf{S}_c^T\mathbf{v}\right) \|_2^2, \tag{72}$$

i.e.,

$$\min_{\mathbf{v}} \ \| \mathbf{D}\mathbf{S}^T\mathbf{y} + \mathbf{D}\mathbf{S}_c^T\mathbf{v} \|_2^2 . \tag{73}$$

From (10), the solution is given by

$$\mathbf{v} = -\left(\mathbf{S}_c\,\mathbf{D}^T\mathbf{D}\,\mathbf{S}_c^T\right)^{-1}\mathbf{S}_c\,\mathbf{D}^T\mathbf{D}\,\mathbf{S}^T\mathbf{y}. \tag{74}$$

Once $\mathbf{v}$ is obtained, the estimate $\hat{\mathbf{x}}$ in (70) can be constructed simply by inserting entries $v(i)$ into $\mathbf{y}$.

An example of least square estimation of missing data using (74) is illustrated in Figure 64. The result is a smoothly interpolated signal.

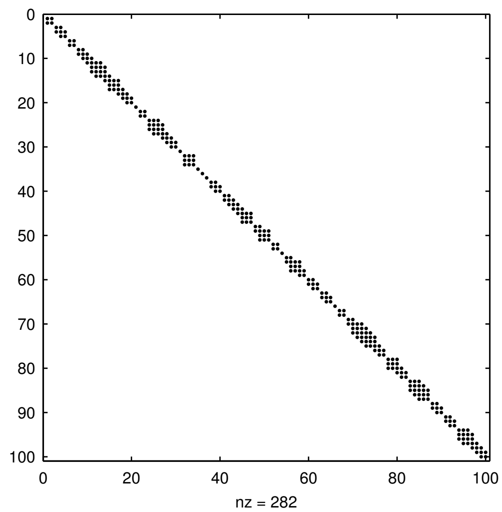


Figure 74: Visualization of the banded matrix $\mathbf{G}$ in (75). All the non-zero values lie near the main diagonal.

We make several remarks.

1. All matrices in (74) are banded, so the computation of $\mathbf{v}$ can be implemented with very high efficiency using a fast solver for banded systems [5]. The banded property of the matrix

$$\mathbf{G} = \mathbf{S}_c\,\mathbf{D}^T\mathbf{D}\,\mathbf{S}_c^T \tag{75}$$

arising in (74) is illustrated in Figure 74.
2. The method does not require the pattern of missing samples to have any particular structure. The missing samples can be distributed quite randomly.
3. This method (74) does not require any regularization parameter λ be specified. However, this derivation does assume the available data, $\mathbf{y}$, is noise free. If $\mathbf{y}$ is noisy, then simultaneous smoothing and missing sample estimation is required (see the Exercises).

Speech de-clipping: In audio recording, if the amplitude of the audio source is too high, then the recorded waveform may suffer from clipping (i.e., saturation). Figure 75 shows a speech waveform that is clipped. All values greater than 0.2 in absolute value are lost due to clipping.

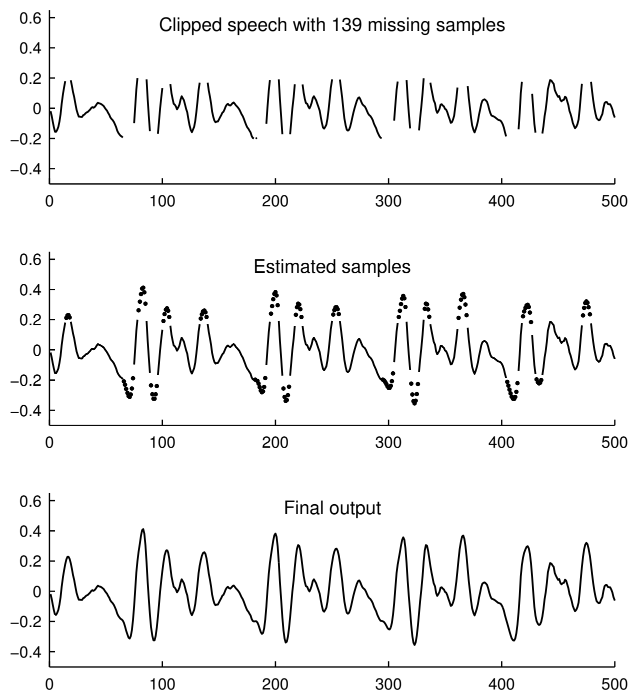


Figure 75: Estimation of speech waveform samples lost due to clipping. The lost samples are estimated by least squares.

To estimate the missing data, we can use the least squares approach given by (74). That is, we fill in the missing data so as to minimize the energy of the derivative of the total signal. In this example, we minimize the energy of the the third derivative. This encourages the filled in data to have the form of a parabola (second order polynomial), because the third derivative of a parabola is zero. In order to use (74) for this problem, we only need to change the matrix $\mathbf{D}$ to the following one. If we define the matrix $\mathbf{D}$ as

$$\mathbf{D} = \begin{bmatrix} 1 & -3 & 3 & -1 & & & & \\ & 1 & -3 & 3 & -1 & & & \\ & & \ddots & & & \ddots & & \\ & & & & 1 & -3 & 3 & -1 \end{bmatrix}, \tag{76}$$

then $\mathbf{Dx}$ is an approximation of the third-order derivative of the signal $\mathbf{x}$.

Using (74) with $\mathbf{D}$ defined in (76), we obtain the signal shown in the Figure 75. The samples lost due to clipping have been smoothly filled in.

Figure 76 shows both, the clipped signal and the estimated samples, on the same axis.

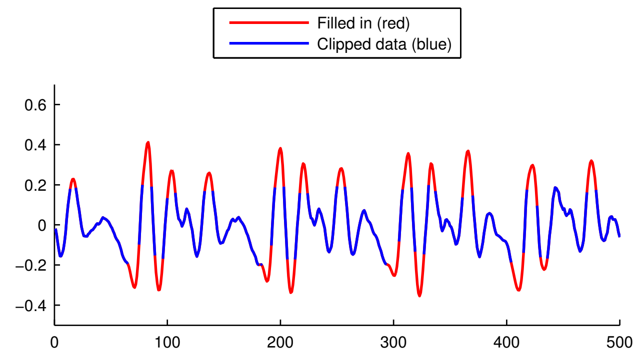


Figure 76: The available clipped speech waveform is shown in blue. The filled in signal, estimated by least squares, is shown in red.

9 Exercises

1. Find the solution $\mathbf{x}$ to the least squares problem:

$$\underset{\mathbf{x}}{min} \ \| \mathbf{y} - \mathbf{A}\mathbf{x} \|_2^2 + \lambda \| \mathbf{b} - \mathbf{x} \|_2^2 \tag{77}$$

2. Show that the solution $\mathbf{x}$ to the least squares problem

$$\underset{\mathbf{x}}{min} \ \lambda_1 \| \mathbf{b}_1 - \mathbf{A}_1\mathbf{x} \|_2^2 + \lambda_2 \| \mathbf{b}_2 - \mathbf{A}_2\mathbf{x} \|_2^2 + \lambda_3 \| \mathbf{b}_3 - \mathbf{A}_3\mathbf{x} \|_2^2 \tag{78}$$

is

$$\begin{aligned} \mathbf{x} = & \left(\lambda_1 \mathbf{A}_1^T \mathbf{A}_1 + \lambda_2 \mathbf{A}_2^T \mathbf{A}_2 + \lambda_3 \mathbf{A}_3^T \mathbf{A}_3\right)^{-1} \\ & \times \left(\lambda_1 \mathbf{A}_1^T \mathbf{b}_1 + \lambda_2 \mathbf{A}_2^T \mathbf{b}_2 + \lambda_3 \mathbf{A}_3^T \mathbf{b}_3\right) \end{aligned} \tag{79}$$

3. In reference to (27), why is $\mathbf{H}^T\mathbf{H} + \lambda\mathbf{I}$ with $\lambda > 0$ invertible even if $\mathbf{H}^T\mathbf{H}$ is not?
4. Show (85).
5. Smoothing. Demonstrate least square smoothing of noisy data. Use various values of λ. What behavior do you observe when λ is very high?
6. The second-order difference matrix (53) was used in the examples for smoothing, deconvolution, and estimating missing samples. Discuss the use of the third-order difference instead. Perform numerical experiments and compare results of 2-nd and 3-rd order difference matrices.
7. System identification. Perform a system identification experiment with varying variance of additive Gaussian noise. Plot the RMSE versus impulse response length. How does the plot of RMSE change with respect to the variance of the noise?
8. Speech de-clipping. Record your own speech and use it to artificially create a clipped signal. Perform numerical experiments to test the least square estimation of the lost samples.
9. Suppose the available data is both noisy and that some samples are missing. Formulate a suitable least squares optimization problem to smooth the data and recover the missing samples. Illustrate the effectiveness by a numerical demonstration (e.g. using Matlab).

10 Vector derivatives

If $f(\mathbf{x})$ is a function of $x_1, \cdots, x_N$, then the derivative of $f(\mathbf{x})$ with respect to $\mathbf{x}$ is the vector of derivatives,

$$\frac{\partial}{\partial \mathbf{x}} f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f(\mathbf{x})}{\partial x_1} \\ \frac{\partial f(\mathbf{x})}{\partial x_2} \\ \vdots \\ \frac{\partial f(\mathbf{x})}{\partial x_N} \end{bmatrix}. \tag{80}$$

This is the gradient of f, denoted ∇f. By direct calculation, we have

$$\frac{\partial}{\partial \mathbf{x}} \mathbf{x}^T \mathbf{b} = \mathbf{b} \tag{81}$$

and

$$\frac{\partial}{\partial \mathbf{x}} \mathbf{b}^T \mathbf{x} = \mathbf{b}. \tag{82}$$

Suppose that $\mathbf{A}$ is a symmetric real matrix, $\mathbf{A}^T = \mathbf{A}$. Then, by direct calculation, we also have

$$\frac{\partial}{\partial \mathbf{x}} \mathbf{x}^T \mathbf{A} \mathbf{x} = 2\mathbf{A}\mathbf{x}. \tag{83}$$

Also,

$$\frac{\partial}{\partial \mathbf{x}} (\mathbf{y} - \mathbf{x})^T \mathbf{A} (\mathbf{y} - \mathbf{x}) = 2\mathbf{A} (\mathbf{x} - \mathbf{y}), \tag{84}$$

and

$$\frac{\partial}{\partial \mathbf{x}} \parallel \mathbf{A}\mathbf{x} - \mathbf{b} \parallel_2^2 = 2\mathbf{A}^T (\mathbf{A}\mathbf{x} - \mathbf{b}). \tag{85}$$

We illustrate (83) by an example. Set $\mathbf{A}$ as the 2×2 matrix,

$$\mathbf{A} = \begin{bmatrix} 3 & 2 \\ 2 & 5 \end{bmatrix}. \tag{86}$$

Then, by direct calculation

$$\mathbf{x}^T \mathbf{A} \mathbf{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 3 & 2 \\ 2 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = 3x_1^2 + 4x_1x_2 + 5x_2^2 \tag{87}$$

so

$$\frac{\partial}{\partial x_1} \left(\mathbf{x}^T \mathbf{A} \mathbf{x} \right) = 6x_1 + 4x_2 \tag{88}$$

and

$$\frac{\partial}{\partial x_2} \left(\mathbf{x}^T \mathbf{A} \mathbf{x} \right) = 4x_1 + 10x_2 \tag{89}$$

Let us verify that the right-hand side of (83) gives the same:

$$2\mathbf{A}\mathbf{x} = 2 \begin{bmatrix} 3 & 2 \\ 2 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \begin{bmatrix} 6x_1 + 4x_2 \\ 4x_1 + 10x_2 \end{bmatrix}. \tag{90}$$

11 The Kth-order difference

The first order difference of a discrete-time signal $x(n)$, $n \in \mathbb{Z}$, is defined as

$$y(n) = x(n) - x(n-1). \tag{91}$$

This is represented as a system with input x and output y,

$$x \;\longrightarrow D \longrightarrow\; y \tag{92}$$

The second order difference is obtained by taking the first order difference twice:

$$x \;\longrightarrow D \longrightarrow D \longrightarrow\; y \tag{93}$$

which give the difference equation

$$y(n) = x(n) - 2\,x(n-1) - x(n-2). \tag{94}$$

The third order difference is obtained by taking the first order difference three times:

$$x \;\longrightarrow D \longrightarrow D \longrightarrow D \longrightarrow\; y \tag{95}$$

which give the difference equation

$$y(n) = x(n) - 3\,x(n-1) + 3\,x(n-2) - x(n-3). \tag{96}$$

In terms of discrete-time linear time-invariant systems (LTI), the first order difference is an LTI system with transfer function

$$D(z) = 1 - z^{-1}. \tag{97}$$

The second order difference has the transfer function

$$D_2(z) = \left(1 - z^{-1}\right)^2 = 1 - 2z^{-1} + z^{-2}. \tag{98}$$

The third order difference has the transfer function

$$D_3(z) = \left(1 - z^{-1}\right)^3 = 1 - 3z^{-1} + 3z^{-2} - z^{-3}. \tag{99}$$

Note that the coefficient come from Pascal's triangle:

				1				
			1		1			
		1		2		1		
	1		3		3		1	
1		4		6		4		1
⋮				⋮				⋮

Table 1

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