

# MATH 350: Introduction to Computational Mathematics

## Chapter V: Least Squares Problems

Greg Fasshauer

Department of Applied Mathematics  
Illinois Institute of Technology

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# Outline

- 1 Motivation and Applications
- 2 The MATLAB Function `polyfit`
- 3 The QR Decomposition
- 4 The SVD



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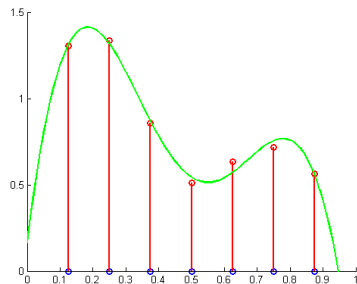
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# Data Fitting

Earlier we discussed the problem of fitting a given set of data by interpolation. However, if the data contain some noise (such as measurement errors in a physical experiment), then we **may not want to exactly fit** the data.

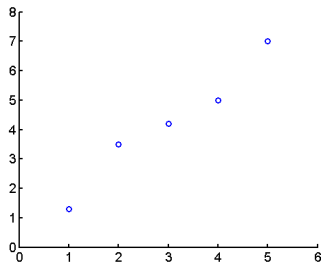
Instead we may want to **approximate the data via a linear least squares (or linear regression) fit**.



## Example

Fit the data

|   |     |     |     |     |     |
|---|-----|-----|-----|-----|-----|
| x | 1   | 2   | 3   | 4   | 5   |
| y | 1.3 | 3.5 | 4.2 | 5.0 | 7.0 |

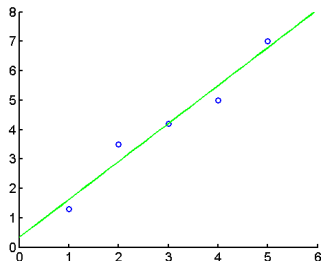


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with a best fitting line.

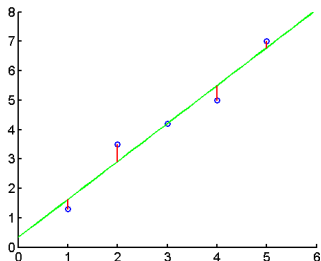


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## Idea

Minimize the sum of the squares of the vertical distances of line from the data points.

# The Normal Equations

Assume the line is of the form

$$L(x) = c_1x + c_2.$$





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If we were to interpolate the data, i.e., enforce

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we would get an **overdetermined** system of linear equations (as soon as  $m > 2$ ):

$$A\mathbf{c} = \mathbf{y},$$

where

$$A = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_m & 1 \end{bmatrix}, \quad \mathbf{c} = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}.$$



## The Normal Equations (cont.)

Minimizing the sums of the squares of the vertical distances from the line to the data points can be expressed as

$$\min_{c_1, c_2} \sum_{i=1}^m [(c_1 x_i + c_2) - y_i]^2$$



## The Normal Equations (cont.)

Minimizing the sums of the squares of the vertical distances from the line to the data points can be expressed as

$$\min_{c_1, c_2} \sum_{i=1}^m [(c_1 x_i + c_2) - y_i]^2 \iff \min_{c_1, c_2} \|\mathbf{A}\mathbf{c} - \mathbf{y}\|_2^2$$



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Since the norm is related to an inner product by

$$\|\mathbf{v}\|_2 = \sqrt{\mathbf{v}^T \mathbf{v}}$$

we want to find the coefficient vector  $\mathbf{c}$  that minimizes

$$(\mathbf{A}\mathbf{c} - \mathbf{y})^T (\mathbf{A}\mathbf{c} - \mathbf{y}) = (\mathbf{c}^T \mathbf{A}^T - \mathbf{y}^T) (\mathbf{A}\mathbf{c} - \mathbf{y})$$



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$$\min_{c_1, c_2} \sum_{i=1}^m [(c_1 x_i + c_2) - y_i]^2 \iff \min_{c_1, c_2} \|\mathbf{Ac} - \mathbf{y}\|_2^2$$

Since the norm is related to an inner product by

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we want to find the coefficient vector  $\mathbf{c}$  that minimizes

$$\begin{aligned} (\mathbf{Ac} - \mathbf{y})^T (\mathbf{Ac} - \mathbf{y}) &= (\mathbf{c}^T \mathbf{A}^T - \mathbf{y}^T) (\mathbf{Ac} - \mathbf{y}) \\ &= \mathbf{c}^T \mathbf{A}^T \mathbf{Ac} - \mathbf{c}^T \mathbf{A}^T \mathbf{y} - \mathbf{y}^T \mathbf{Ac} + \mathbf{y}^T \mathbf{y} \end{aligned}$$



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The last equality holds because  $\mathbf{c}^T \mathbf{A}^T \mathbf{y} = \mathbf{y}^T \mathbf{A}\mathbf{c}$  is a scalar quantity (and therefore equal to its transpose).



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From Calculus we know that a necessary<sup>1</sup> condition for the minimum is that the partials with respect to  $c_1$  and  $c_2$  are zero.

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In vector notation this means

$$2A^T A \mathbf{c} - 2A^T \mathbf{y} = 0$$

or

$$A^T A \mathbf{c} = A^T \mathbf{y}.$$

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*The normal equations characterize the **least squares solution** of the system  $A \mathbf{c} = \mathbf{y}$ . They are important for theoretical purposes and provide simple notation.*

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### Remark

*The normal equations characterize the **least squares solution** of the system  $A \mathbf{c} = \mathbf{y}$ . They are important for theoretical purposes and provide simple notation.*

*However, they are not recommended for serious computations!*

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# Do not compute with the normal equations!

## Example

Fit the data

|   |    |       |       |       |       |     |
|---|----|-------|-------|-------|-------|-----|
| x | 10 | 10.2  | 10.4  | 10.6  | 10.8  | 11  |
| y | 0  | 0.004 | 0.016 | 0.036 | 0.064 | 0.1 |

with a quadratic polynomial  $Q(x) = c_1x^2 + c_2x + c_3$ .

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Note that the data actually come from the function

$$f(x) = \frac{x^2}{10} - 2x + 10,$$

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The MATLAB script `LSQquad.m` illustrates what happens when we use the normal equations to solve the problem in single and double precision.

The derivation of the normal equations works **analogously** for any **linear approximation** of the form

$$P(x) = c_1 b_1(x) + c_2 b_2(x) + \dots + c_n b_n(x),$$

where  $\{b_1, \dots, b_n\}$  is some set of **basis functions** we want to compute the least squares fit with. This could be polynomials, trigonometric functions, logarithms, exponentials, etc.





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The matrix  $A$  is a **Vandermonde-like matrix** of the form

$$A = \begin{bmatrix} b_1(x_1) & b_2(x_1) & \dots & b_n(x_1) \\ b_1(x_2) & b_2(x_2) & \dots & b_n(x_2) \\ \vdots & \vdots & & \vdots \\ b_1(x_m) & b_2(x_m) & \dots & b_n(x_m) \end{bmatrix}.$$

Usually, this is a **tall and skinny matrix**, i.e.,  $m > n$ . In this case we have **more data points than unknown coefficients**, i.e., an **over-determined linear system**.



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The normal equations are always given by

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## Question

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## Example

Instead of using the monomial basis  $\{x^2, x, 1\}$  as we did in LSQquad.m, we can use the **orthogonal basis**  $\left\{ \left(x - \frac{21}{2}\right)^2 - \frac{7}{60}, x - \frac{21}{2}, 1 \right\}$ .



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The MATLAB script `LSQquadOrtho.m` illustrates what happens when we use the normal equations based on an orthogonal basis to solve the previous fitting problem in single precision.



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The **QR decomposition** (see below) produces an orthogonal matrix that helps us solve the least squares problem in a stable way.



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The two commands required for this are

`p = polyfit(x, y, n)`: returns the coefficients  $p$  of the degree  $n$  polynomial

$$p(x) = p(1)x^n + p(2)x^{n-1} + \dots + p(n)x + p(n+1)$$

that provides the best least squares fit to the data in  $x$  and  $y$ .



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The MATLAB script `PolyfitDemo.m` illustrates the use of these two functions for the data from the previous example and for the same data contaminated with 10% noise.



The MATLAB function `censusgui` from [NCM] illustrates the use of normalized data for polynomial least squares fitting of U.S. population data.

It also uses `pchip` along with `spline` fitting, and an exponential fit of the type

$$y = ce^{\alpha x}.$$



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### Remark

*If you are interested in **statistics**, then `[p, S] = polyfit(x, y, n)` will also provide information for **error bounds on the prediction** in `S`, and `[p, S, mu] = polyfit(x, y, n)` will produce the coefficients of a fitting polynomial in the normalized variable  $\hat{x} = (x - \mu)/\sigma$ , where  $\mu = \text{mu}(1)$  is the **mean** of the data sites `x` and  $\sigma = \text{mu}(2)$  is the **standard deviation**.*



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## Theorem

Every real  $m \times n$  matrix  $A$  has a *QR decomposition*

$$A = QR,$$

where  $Q$  is an  $m \times m$  *orthogonal matrix* and  $R$  is an  $m \times n$  upper triangular matrix.



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There are many different ways in which the matrices  $Q$  and  $R$  can be found. E.g., one can use

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All of these are discussed in MATH 477. We will only investigate the *use* of the QR decomposition.

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Note that this implies that

$$Q^{-1} = Q^T \quad \text{— a very handy property.}$$





## Orthogonal Matrices (cont.)

### Example

Verify that the matrix

$$Q = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} & \frac{-1}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{3}} & \frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{3}} & \frac{1}{\sqrt{6}} \end{bmatrix}$$

is an orthogonal matrix.

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We need to verify that

$$\begin{aligned} \mathbf{q}_1^T \mathbf{q}_2 &= 0, & \mathbf{q}_1^T \mathbf{q}_3 &= 0, & \mathbf{q}_2^T \mathbf{q}_3 &= 0, \\ \mathbf{q}_1^T \mathbf{q}_1 &= 1, & \mathbf{q}_2^T \mathbf{q}_2 &= 1, & \mathbf{q}_3^T \mathbf{q}_3 &= 1. \end{aligned}$$

Note that the conditions in the second row are equivalent to  $\|\mathbf{q}_i\|_2 = 1$ ,  $i = 1, 2, 3$ .

**Example** (cont.)

Columns are pairwise perpendicular:

$$\mathbf{q}_1^T \mathbf{q}_2 = \left[ \frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}} \right] \begin{bmatrix} \frac{1}{\sqrt{3}} \\ \frac{2}{\sqrt{6}} \\ \frac{-1}{\sqrt{3}} \end{bmatrix}$$



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## Orthogonal Matrices (cont.)

Another important property of any  $m \times m$  orthogonal matrix  $Q$  is that it leaves the **2-norm invariant**, i.e., for any  $m$ -vector  $\mathbf{x}$  we have

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### Remark

*In fact, orthogonal matrices/transformations represent either a **rotation** (if  $\det Q = 1$ ) or a **reflection** ( $\det Q = -1$ ), i.e., a length-preserving (or isometric) geometric transformation.*

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### Remark

*In fact, orthogonal matrices/transformations represent either a **rotation** (if  $\det Q = 1$ ) or a **reflection** ( $\det Q = -1$ ), i.e., a length-preserving (or isometric) geometric transformation. Angles are also preserved (just compare  $(Q\mathbf{x})^T(Q\mathbf{y})$  with  $\mathbf{x}^T \mathbf{y}$ ).*

Consider first the square non-singular linear system  $A\mathbf{x} = \mathbf{b}$ , and assume that  $A$  has the QR decomposition  $A = QR$ .



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This is an **upper triangular system** for the unknown vector  $\mathbf{x}$  which can be easily solved by back substitution (note a certain similarity with the procedure used with the LU decomposition earlier).





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This is an **upper triangular system** for the unknown vector  $\mathbf{x}$  which can be easily solved by back substitution (note a certain similarity with the procedure used with the LU decomposition earlier).

In fact, QR decomposition is in most cases the **preferred method for the solution of linear systems**. It provides a **good balance of numerical stability** (better than LU) **and efficiency** (worse than LU).



Recall that the least squares solution of the overdetermined linear system  $\mathbf{A}\mathbf{c} = \mathbf{y}$  is given by the coefficient vector  $\mathbf{c}$  that minimizes the norm of the 2-norm residual  $\|\mathbf{A}\mathbf{c} - \mathbf{y}\|_2$ .



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Finally, in the overdetermined system case (with  $m > n$ ) the last  $m - n$  rows of the upper triangular matrix  $R$  are in fact all zero.

Therefore, the least squares solution of  $A\mathbf{c} = \mathbf{y}$  is given by the solution of the square upper triangular system (provided  $A$  has full (column) rank  $n$ )

$$\hat{R}\mathbf{c} = \mathbf{z},$$

where  $\hat{R} = R(1:n, 1:n)$  and  $\mathbf{z} = Q^T(1:n, :)\mathbf{y}$ .



## Example

Again we use the data

|   |    |       |       |       |       |     |
|---|----|-------|-------|-------|-------|-----|
| x | 10 | 10.2  | 10.4  | 10.6  | 10.8  | 11  |
| y | 0  | 0.004 | 0.016 | 0.036 | 0.064 | 0.1 |

(without and with noise) and fit with a quadratic polynomial  
 $P(x) = c_1x^2 + c_2x + c_3$ .



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The MATLAB script `LSQquadQR.m` illustrates how we can use the method described above based on the QR decomposition of  $A$  to obtain the fit.



# Outline

- 1 Motivation and Applications
- 2 The MATLAB Function `polyfit`
- 3 The QR Decomposition
- 4 The SVD**



## Theorem

Let  $A$  be a complex  $m \times n$  matrix.  $A$  has a *singular value decomposition* of the form

$$A = U\Sigma V^*,$$

where  $\Sigma$  is a uniquely determined  $m \times n$  (real) diagonal matrix,  $U$  is an  $m \times m$  unitary matrix, and  $V$  is an  $n \times n$  unitary matrix.



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## Remark

- The entries  $\sigma_i$  of the diagonal matrix  $\Sigma$  are the *singular values* of  $A$  (recall our earlier discussion of the matrix 2-norm).
- Note that this theorem guarantees that *every matrix can be diagonalized!*
- The theorem is very general. If  $A$  is a *real* matrix, then “unitary” translates to “*orthogonal*” and “ $*$ ” (Hermitian conjugate) to “ $T$ ”.

Using the SVD to solve  $\|A\mathbf{c} - \mathbf{y}\|_2 \rightarrow \min$

Assume  $A$  is real  $m \times n$ ,  $m \geq n$ , and  $\text{rank}(A) = r = n$ .



## Using the SVD to solve $\|A\mathbf{c} - \mathbf{y}\|_2 \rightarrow \min$

Assume  $A$  is real  $m \times n$ ,  $m \geq n$ , and  $\text{rank}(A) = r = n$ .

Compute reduced SVD

$$A = \hat{U}\hat{\Sigma}V^T,$$

with  $\hat{U} = U(:, 1:r)$  an  $m \times r$  real matrix with orthogonal columns, real diagonal  $\hat{\Sigma} = \Sigma(1:r, 1:r)$ , and real orthogonal  $r \times r$  matrix  $V$ .





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More details are provided in Chapters 5 and 10 of [NCM] as well as in MATH 477.



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


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- A new algorithm that very efficiently finds all singular values with high relative accuracy was found recently by [Drmač & Veselić]. 

# References I



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New fast and accurate Jacobi SVD algorithm: Parts I and II.

SIAM J. Matrix Anal. Appl. **29** (2008), 1322–1362.



# Outline

## 5 The SVD



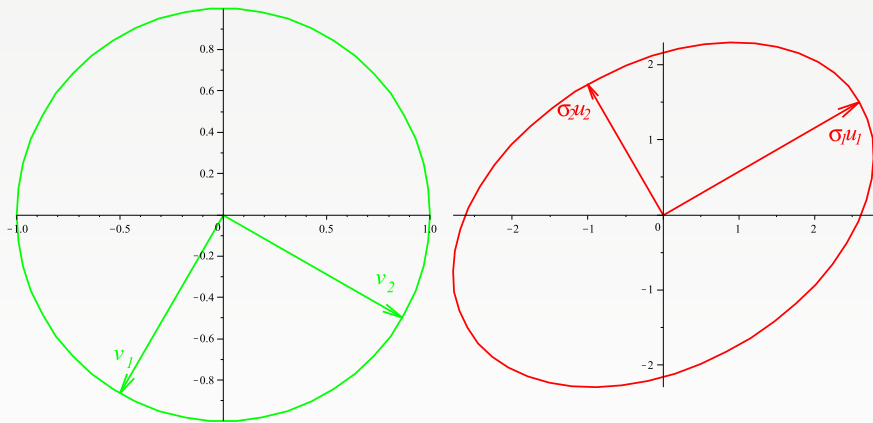


Figure: ON bases for row space and column space of  $A$ .



## Theorem

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Moreover, the best 2-norm approximation of rank  $\nu$  ( $0 \leq \nu \leq r$ ) to  $A$  is given by

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This theorem is very useful for applications such as image compression and is illustrated in the MATLAB script `SVD_movie.m` (see also `imagesvd.m` from [NCM]).

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