Computational method and numerical algorithms: Lecture 5

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Contents

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4.1 Inconsistent systems of equations

Let's consider the following system of equations:

$$\begin{aligned} x_1 + x_2 &= 2, \\ x_1 - x_2 &= 1, \\ x_1 + x_2 &= 3. \end{aligned}$$

It is clear that this system of equations has no solutions.
A system of equations with no solution is called **inconsistent**.
Alternatively, we can find a solution that makes the equations as "accurate" as possile.
How to quantify the accuracy of a solution?

Euclidean distance

We rewrite the previous equations in the following vector form

$$v_1 x_1 + v_2 x_2 = b,$$

where

$$v_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, v_2 = \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix} b = \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix}$$

We know that,

$$v_1 x_1 + v_2 x_2, x_1, x_2 \in \mathbb{R}$$

forms a plane Π in $\mathbb{R}^3$. If vector $b \in \mathbb{R}^3$ is on the plane, then the above equation has a unique solution.
What if b is outside the plane?

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Least Squares

We hope to find a unique solution $\bar{x} = (\bar{x}_1, \bar{x}_2)$ such that the following function

$$||b - (v_1 x_1 + v_2 x_2)||_2$$

attains its minimum at $x_1 = \bar{x}_1$ and $x_2 = \bar{x}_2$?
The optimal solution $\bar{x}$ in fact satisfies

$$b - (v_1\bar{x}_1 + v_2\bar{x}_2) \perp \text{Plane} \quad \Pi = \{x_1 v_1 + x_2 v_2 : x_1, x_2 \in \mathbb{R}\},$$

i.e., for all $x_1, x_2 \in \mathbb{R}$,

$$(x_1 v_1 + x_2 v_2)^T [b - (v_1\bar{x}_1 + v_2\bar{x}_2)] = 0 \to [v_1, v_2][b - (v_1\bar{x}_1 + v_2\bar{x}_2)] = 0.$$

In general, when we need to solve $Ax = b$ with $A \in \mathbb{R}^{m\times n}$ and $b \in \mathbb{R}^m$ and $m > n$, we can solve the following **Least Squares** problem

$$\min_{x\in\mathbb{R}^n} ||b - Ax||_2, \text{ or } \quad \min_{x\in\mathbb{R}^n} ||Ax - b||_2^2.$$

Accordingly, we expect that the optimal solution $\bar{x}$ satisfies

$$b - A\bar{x} \perp \text{Super Plane} \quad \Pi = \{Ax \in \mathbb{R}^m : x \in \mathbb{R}^n\},$$

i.e.,

$$(Ax)^T(b - A\bar{x}) = 0, \quad \forall x \in \mathbb{R}^n \to A^T(b - A\bar{x}) = 0.$$

Can we derive that above result by Calculus?

Normal Equations

Revisit the least squares problem,

$$\min_{x\in\mathbb{R}^n}\left(y(x)=||b-Ax||_2^2\right),$$

where $A\in\mathbb{R}^{m\times n}$ and $b\in\mathbb{R}^m$. Suppose that $y(x)$ has a minimum value at $x=\bar{x}$. Then, what does Calculus tell us?

$$\mathcal{J}_x y(x)|_{x=\bar{x}} = \quad .$$

This directly gives rise to the following **normal equations**

Its solution $\bar{x}$ minimizes the Euclidean length of the residual $r=b-Ax$. Different types of errors:

- **2-norm error:** $||r||_2=||b-A\bar{x}||$.
- **Sqaured error:** $\mathrm{SE}=||r||_2^2$.
- **Root mean squared error:** $\mathrm{RMSE}=\sqrt{SE/m}$.

Normal Equations

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$$\mathcal{J}_x y(x)|_{x=\bar{x}}=0.$$

This directly gives rise to the following **normal equations**

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Normal Equations

Revisit the least squares problem,

$$\min_{x \in \mathbb{R}^n} \left(y(x) = ||b - Ax||_2^2 \right),$$

where $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$. Suppose that $y(x)$ has a minimum value at $x = \bar{x}$. Then, what does Calculus tell us?

$$\mathcal{J}_x y(x)|_{x=\bar{x}} = 0.$$

This directly gives rise to the following **normal equations**

$$A^T(b - A\bar{x}) = 0 \to A^T A\bar{x} = A^T b.$$

Its solution $\bar{x}$ minimizes the Euclidean length of the residual $r = b - Ax$. Different types of errors:

- **2-norm error:** $||r||_2 = ||b - A\bar{x}||$.
- **Sqaured error:** $\mathrm{SE} = ||r||_2^2$.
- **Root mean squared error:** $\mathrm{RMSE} = \sqrt{SE/m}$.

Example 1. Use the normal equations to find the least squares solution of the inconsistent system

$$
\begin{aligned}
x_1 + x_2 &= 2, \\
x_1 - x_2 &= 1, \\
x_1 + x_2 &= 3.
\end{aligned}
$$

Sol. We have

$$A = \begin{bmatrix} 1 & 1 \\ 1 & -1 \\ 1 & 1 \end{bmatrix}, \quad b = \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix}.$$

Thus, the components of the normal equations are

$$A^T A = \begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix}, \quad A^T b = \begin{bmatrix} 6 \\ 4 \end{bmatrix}.$$

We can solve

$$\begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix} \bar{x} = \begin{bmatrix} 6 \\ 4 \end{bmatrix} \rightarrow \bar{x} = \begin{bmatrix} 7/4 \\ 3/4 \end{bmatrix}.$$

Thus, the residual vector

$$r = b - A\bar{x} = \begin{bmatrix} -0.5 \\ 0 \\ 0.5 \end{bmatrix}, \quad ||r||_2 = \sqrt{0.5} \approx 0.707$$

$$\mathrm{SE} = ||r||_2^2 = 0.5, \quad \mathrm{RMSE} = \sqrt{\mathrm{SE}/m} = 1/\sqrt{6} \approx 0.408.$$

Fitting models to data

Let $(x_1, y_1), \dots (x_m, y_m)$ be a set of points in the plane. Given a fixed class of models, such as all lines $y = c_1 + c_2 x$, we hope to find the specific instance of the model that best fits the data points in the 2-norm.

Specifically, once we find out the model, then checking this model at the m points we get an error vector, $e = [e_1, e_2, \dots, e_m]$. The best-fitting model has the following property the 2-norm of e, i.e.,

$$||e||_2 = \sqrt{e_1^2 + e_2^2 + \cdots + e_m^2}$$

attains its minimum.

Best-fitting line

Example 1. Find the line that best fits the three data points $(x, y) = (1, 2), (-1, 1)$ and $(1, 3)$.
Sol. Suppose the line is $y = c_1 + c_2 x$, then we hope that

$$
\begin{aligned}
e_1 &= c_1 + 1 \cdot c_2 - 2 = 0, \\
e_2 &= c_1 + (-1) \cdot c_2 - 1 = 0, \\
e_3 &= c_1 + 1 \cdot c_2 - 3 = 0.
\end{aligned}
$$

This then gives rise to a least squares problem, we can solve the normal equations to get $c_1 = 7/4, c_2 = 3/4$. Consequently, the best-fitting line is $y = 7/4 + 3x/4$. Then, we get the following table regarding residuals

x	y	line	error
1	2	2.5	$e_1 = -0.5$
-1	1	1.0	$e_2 = 0.0$
1	3	2.5	$e_3 = 0.5.$

Then the SE is $(-0.5)^2 + 0.5^2 = 0.5$ and the RMSE $= 1/\sqrt{6}$.

Best-fitting parabola

Example 2. Find the parabola that best fits the four data points $(-1,1),(0,0),(1,0)$, and $(2,-2)$.

Sol. Suppose the parabola is $y = c_1 + c_2 x + c_3 x^2$, then we hope that

$$\begin{cases} e_1 = c_1 + (-1)c_2 + (-1)^2 c_3 - 1 = 0 \\ e_2 = c_1 + (0)c_2 + (0)^2 c_3 - 0 = 0 \\ e_3 = c_1 + (1)c_2 + (1)^2 c_3 - 0 = 0 \\ e_4 = c_1 + 2c_2 + 2^2 c_3 - (-2) = 0. \end{cases} \rightarrow \begin{bmatrix} 1 & -1 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

However, this cannot have a solution. Instead, we hope 2-norm of $e = [e_1, e_2, e_3, e_4]$ attains its minimum, we need to solve the related least squares problem again. Thus, we solve the normal equations

$$\begin{bmatrix} 4 & 2 & 6 \\ 2 & 6 & 8 \\ 6 & 8 & 18 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} -1 \\ -5 \\ -7 \end{bmatrix} \rightarrow \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} 0.45 \\ -0.65 \\ -0.25 \end{bmatrix}.$$

Thus, the parabolar is $y = 0.45 - 0.65t - 0.25t^2$. The residual errors are

x	y	parabola	error
-1	1	0.85	$e_1 = 0.15$
0	0	0.45	$e_2 = -0.45$
1	0	-0.45	$e_3 = 0.45.$
2	-2	-1.85	$e_4 = -0.15.$

SE is $e_1^2 + e_2^2 + e_3^2 + e_4^2 = 0.45$, and RMSE$= \sqrt{0.45}/\sqrt{4} \approx 0.335$.

Fitting data by least squares

Given a set of m data points $(x_1, y_1), \ldots, (x_m, y_m)$.

1. Choose a model.
2. Force the model to fit the data.
3. Solve the normal equations.

Condition Number of Normal Equations

When fitting a given set of data points, shall higher degree polynomials provide better-fitting model?

The answer is

Example 3. Let $x_1 = 2.0, x_2 = 2.2, x_3 = 2.4, \ldots, x_{11} = 4.0$. Set $y_i = \sum_{n=0}^{7} x_i^n$ for $1 \leq i \leq 11$. Use the normal equations to find the least squares polynomial $P(x) = \sum_{n=1}^{8} c_n x^{n-1}$ fitting (x_i, y_i).

Condition Number of Normal Equations

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When fitting a given set of data points, shall higher degree polynomials provide better-fitting model?
The answer is NO.
Example 3. Let $x_1 = 2.0, x_2 = 2.2, x_3 = 2.4, \ldots, x_{11} = 4.0$. Set $y_i = \sum_{n=0}^{7} x_i^n$ for $1 \leq i \leq 11$. Use the normal equations to find the least squares polynomial $P(x) = \sum_{n=1}^{8} c_n x^{n-1}$ fitting (x_i, y_i).

4.3 QR Factorization

Since Normal Equations can have ill-conditioned coefficient matrix, we here give a technique that is more preferred to Normal Equations for solving least squares problem.

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Gram-Schmidt orthogonalization and least squares

Let $A_1, \ldots, A_n$ be linearly independent vectors in $\mathbb{R}^m$. Thus $n \le m$. The **Gram-Schmidt orthogonalization** procedure turn the above vectors into n unit vectors orthogonal to each other.
We first turn A_1 into a unit vector,

$$y_1 = A_1, \quad q_1 = \frac{y_1}{||y_1||_2}.$$

To find the next unit vector that is orthogonal to y_1, we set

$$y_2 = A_2 - q_1(q_1^T A_2), \quad q_2 = \frac{y_2}{||y_2||_2}.$$

We can check

$$y_2^T q_1 = A_2^T q_1 - q_1^T q_1(q_1^T A_2) = A_2^T q_1 - q_1^T A_2 = 0 \to q_2^T q_1 = 0.$$

To find the j-th vector q_j from A_j, $q_1, \ldots, q_{j-1}$, we set

$$y_j = A_j - \sum_{l=1}^{j-1} q_l(q_l^T A_j), \quad q_j = \frac{y_j}{||y_j||_2}.$$

One easily check that for $i = 1, \ldots, j-1$,

$$y_j^T q_i = A_j^T q_i - \sum_{l=1}^{j-1} q_l^T q_i(q_l^T A_j) = A_j^T q_i - q_i^T A_j = 0 \to q_j^T q_i = 0.$$

Consequently, we get all $q_1, q_2, \ldots, q_n$ that are pairwise orthogonal.

Reduced QR Factorization

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Let

$$r_{jj} = ||y_j||_2, r_{ij} = q_i^T A_j,$$

then

$$A_j = \sum_{i=1}^{j-1} q_i(q_i^T A_j) + y_j = \sum_{i=1}^{j-1} r_{ij} q_i + r_{jj} q_j = \sum_{i=1}^{j} r_{ij} q_j, \quad j = 1, \ldots, n.$$

In matrix form, we get

$$[A_1|A_2|\cdots|A_n] = [q_1|q_2|\cdots|q_n] \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & \cdots & r_{2n} \\ & & \ddots & \vdots \\ & & & r_{nn} \end{bmatrix}.$$

Or, $A = QR$, where Q consists of pairwise orthonormal vectors such that $Q^T Q = I_n$ and R is an upper triangular matrix. Such a decomposition is the so-called **reduced QR Factorization**. Can $r_{jj} = 0$ Here?

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Example 1. Find the reduced QR factorization by applying Gram-Schmidt orthogonalization to the columns of

$$A = \begin{bmatrix} 1 & -4 \\ 2 & 3 \\ 2 & 2 \end{bmatrix}.$$

Classic Gram-Schmidt orthogonalization

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Let $A_j, j = 1, \ldots, n$ be linearly independent vectors:
for $j = 1, 2, \ldots, n$
  $y = A_j$
  for $i = 1, 2, \ldots, j-1$
    $r_{ij} = q_i^T A_j$
    $y = y - r_{ij} q_i$
  end
  $r_{jj} = ||y||_2$
  $q_j = y / r_{jj}$
end
Computational Complexity:

Full QR Factorization

If we add $m-n$ vectors $\{A_j\}_{j=n+1}^{m}$ to the set of $\{A_j\}_{j=1}^{n}$ so that $\{A_j\}_{j=1}^{m}$ form a basis of $\mathbb{R}^m$, and then do the classic GS orthogonalization, we get

$$[A_1|A_2|\ldots|A_m] = [q_1|q_2|\ldots|q_m]\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} & \cdots & r_{1m} \\ & r_{22} & \cdots & r_{2n} & \cdots & r_{2m} \\ & & \ddots & \vdots & \ddots & \\ & & & r_{nn} & \cdots & r_{nm} \\ & & & & \ddots & \vdots \\ & & & & & r_{mm} \end{bmatrix}$$

Then, we easily see that

$$[A_1|A_2|\ldots|A_n] = QR = [q_1|q_2|\ldots|q_m]\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & \cdots & r_{2n} \\ & & \ddots & \vdots \\ & & & r_{nn} \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix},$$

which is the so-called **Full QR Factorization**.

Example 2. Find the full QR factorization by applying Gram-Schmidt orthogonalization to the columns of

$$A = \begin{bmatrix} 1 & -4 \\ 2 & 3 \\ 2 & 2 \end{bmatrix}.$$

Orthogonal matrix

$Q = [q_1|q_2|\dots|q_m] \in \mathbb{R}^{m\times m}$. Since $q_1, q_2, \cdots, q_m$ are orthonormal to each other, we easily see that

$$Q^T Q = \quad .$$

In other words, $Q^T = Q^{-1}$. Matrices with such a property are called orthogonal matrices.

Prop. 1 If Q is an $m \times m$ orthogonal matrix, then for any $b \in \mathbb{R}^m$, $||Qb||_2 = ||b||_2$.

Proof.

Orthogonal matrix

$Q = [q_1|q_2|\dots|q_m] \in \mathbb{R}^{m\times m}$. Since $q_1, q_2, \cdots, q_m$ are orthonormal to each other, we easily see that

$$Q^T Q = I_m.$$

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Prop. 1 If Q is an $m \times m$ orthogonal matrix, then for any $b \in \mathbb{R}^m$, $||Qb||_2 = ||b||_2$.
Proof.

Least Squares by QR Factorization

Recall Full QR Factorization:

$$[A_1|A_2|\ldots|A_n] = QR = [q_1|q_2|\ldots|q_m]\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & \cdots & r_{2n} \\ & & \ddots & \vdots \\ & & & r_{nn} \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}$$

Least Squares Problem: Given $A \in \mathbb{R}^{m\times n}$, $b \in \mathbb{R}^m$, find $x \in \mathbb{R}^n$ such that $||Ax - b||_2 = ||QRx - b||_2 = ||Rx - Q^T b||_2$ attains the minimum. Let $d = Q^T b$, then the residual vector

$$\left[\begin{array}{c} e_1 \\ \vdots \\ e_n \\ \hline e_{n+1} \\ \vdots \\ e_m \end{array}\right] = \left[\begin{array}{cccc} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & \cdots & r_{2n} \\ & & \ddots & \vdots \\ & & & r_{nn} \\ \hline 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 \end{array}\right] \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} - \left[\begin{array}{c} d_1 \\ \vdots \\ d_n \\ \hline d_{n+1} \\ \vdots \\ d_m \end{array}\right]$$

We cannot let $e_{n+1}, \ldots, e_m$ vanish by properly selecting x. Since

$$[e_{n+1}, \ldots, e_m] = -[d_{n+1}, \ldots, d_m].$$

Therefore, we can only enforce

$$\begin{bmatrix} e_1 \\ \vdots \\ e_n \end{bmatrix} = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & \cdots & r_{2n} \\ & & \ddots & \vdots \\ & & & r_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} - \begin{bmatrix} d_1 \\ \vdots \\ d_n \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}$$

Thus, we get the following approach to solve the least squares problem. Given the $m \times n$ inconsistent system

$$Ax = b,$$

find the full QR factorization $A = QR$ and set:

1. $\hat{R}$ = upper $n \times n$ submatrix of R;
2. $\hat{d}$ = upper n entries of $d = Q^T b$.

Solve $\hat{R}\bar{x} = \hat{d}$ for the least squares solution $\bar{x}$.

Example 3. Use the full QR factorization to solve the least squares prolem

$$\begin{bmatrix} 1 & -4 \\ 2 & 3 \\ 2 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} -3 \\ 15 \\ 9 \end{bmatrix}$$

Example 4. Use the QR factorization to solve a previous least squares problem: Let $x_1 = 2.0, x_2 = 2.2, x_3 = 2.4, \ldots, x_{11} = 4.0$. Set $y_i = \sum_{n=0}^{7} x_i^n$ for $1 \leq i \leq 11$. Use the normal equations to find the least squares polynomial $P(x) = \sum_{n=1}^{8} c_n x^{n-1}$ fitting (x_i, y_i).

Modified Gram-Schmidt orthogonalization

Let $A_j, j = 1, \ldots, n$ be linearly independent vectors:

for $j = 1, 2, \ldots, n$
  $y = A_j$
  for $i = 1, 2, \ldots, j-1$
    $r_{ij} = q_i^T A_j$
    $y = y - r_{ij} q_i$
  end
  $r_{jj} = ||y||_2$
  $q_j = y / r_{jj}$
end

Let $A_j, j = 1, \ldots, n$ be linearly independent vectors:

for $j = 1, 2, \ldots, n$
  $y = A_j$
  for $i = 1, 2, \ldots, j-1$
    $r_{ij} = q_i^T y$
    $y = y - r_{ij} q_i$
  end
  $r_{jj} = ||y||_2$
  $q_j = y / r_{jj}$
end

Example 4. Compare the results of classic GS and modified GS, computed in double precision, on the matrix of almost-parallel vectors

$$A = \begin{bmatrix} 1 & 1 & 1 \\ \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \delta \end{bmatrix},$$

where $\delta = 10^{-10}$.

Householder reflectors

A **Householder reflector** is an orthogonal matrix that reflects all m-vectors through an $m-1$ dimensional plane.

Theorem. Let x and w be vectors with $||x||_2 = ||w||_2$ and define $v = w - x$. Then $H = I - 2vv^T/v^Tv$ is a symmetric orthogonal matrix and $Hx = w$.

Proof.

Example 1. Let $x = [3, 4]$ and $w = [5, 0]$. Find a Householder reflector H that satisfies $Hx = w$.

Use Householder reflectors to find QR

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Example 2. Use Householder reflectors to find the QR factorization of

$$\begin{bmatrix} 3 & 1 \\ 4 & 3 \end{bmatrix}.$$

Example 3. Use Householder reflectors to find the QR factorization of

$$\begin{bmatrix} 1 & -4 \\ 2 & 3 \\ 2 & 2 \end{bmatrix}.$$

General Case

How can we use Householder reflectors to find QR Factorization of an $m \times n$ matrix A?

Contents

Assignment IV

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Assignment V:
P199, Computer Problems: 1.
P225, Computer Problems: 1,3.
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