AFRICAN INSTITUTE FOR MATHEMATICAL SCIENCES, AIMS RWANDA

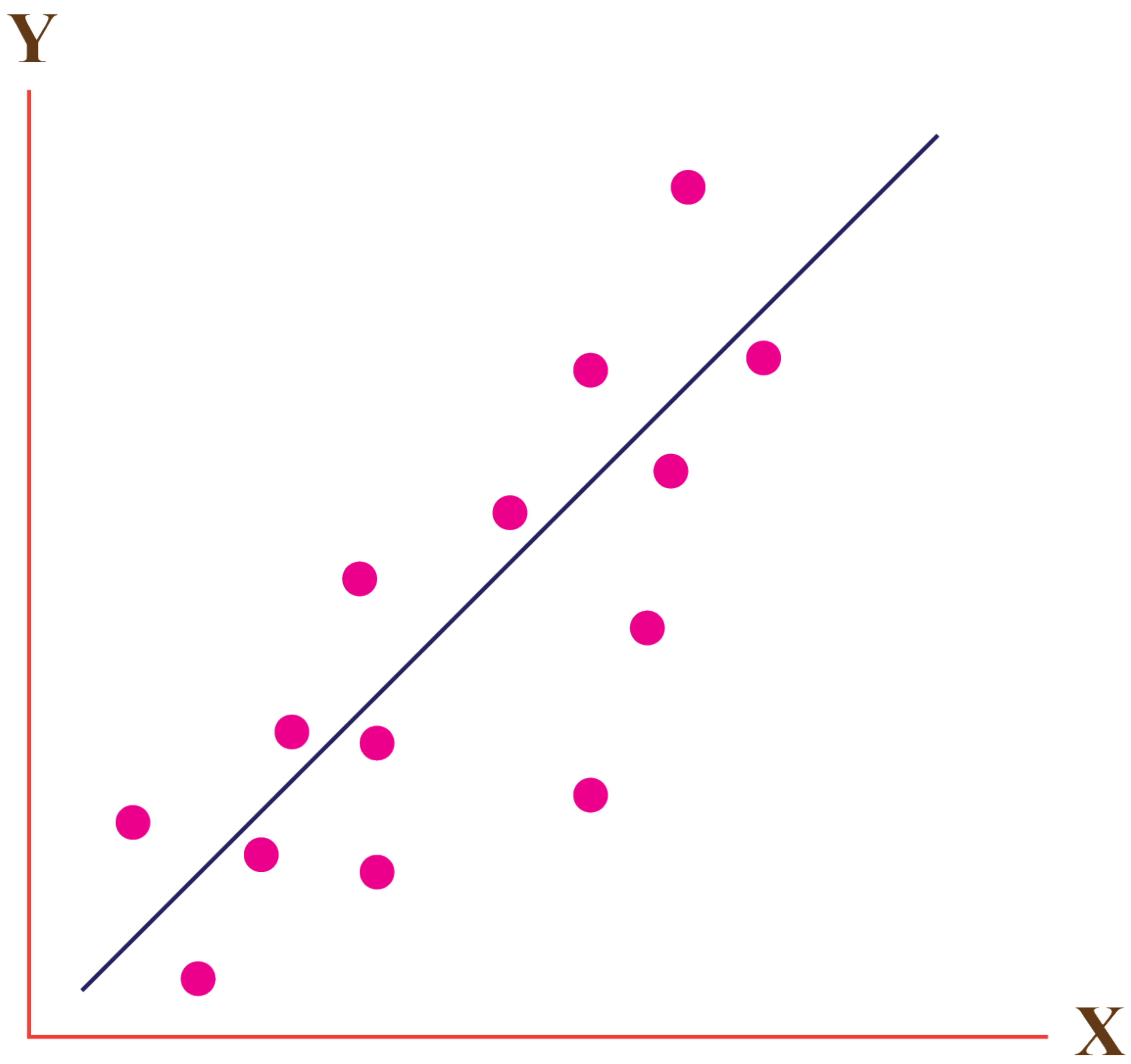
AIMS | African Institute for Mathematical Sciences RWANDA

THE LEAST SQUARES PROBLEM

Prof. Franck Kalala Mutombo
University of Lubumbashi

THE LEAST SQUARES PROBLEM

THE DISCRETE LEAST SQUARES PROBLEM



LS

THE LEAST SQUARES PROBLEM

THE DISCRETE LEAST SQUARES PROBLEM

A task that occurs frequently in scientific investigations is that of finding a straight line that "fits" some set of data points. Typically we have a fairly large number of points (t_i, y_i), $i = 1, \ldots, n$, collected from some experiment, and often we have some theoretical reason to believe that these points should lie on a straight line.

we seek a linear function $p(t) = a_0 + a_1 t$ such that $p(t_i) = y_i$, $i = 1, \ldots, n$.

In practice of course the points will deviate from a straight line, so it is impossible to find a linear $p(t)$ that passes through all of them. Instead we settle for a line that fits the data well, in the sense that the errors

$$|y_i - p(t_i)| \qquad i = 1, \ldots, n$$

are made as small as possible.

THE LEAST SQUARES PROBLEM

THE DISCRETE LEAST SQUARES PROBLEM

It is generally impossible to find a p for which all of the numbers $|y_i - p(t_i)|$ are simultaneously minimized, so instead we seek a p that strikes a good compromise.

Specifically, let $r = [r_1, \cdots, r_n]^T$ denote the vector of residuals $r_i = y_i - p(t_i)$. We can solve our problem by choosing a vector norm $\|\cdot\|$ and taking our compromise function to be that p for which $\|r\|$ is made as small as possible. Of course the solution depends on the choice of norm. For example, if we choose the Euclidean norm, we minimize the quantity

$$\|r\|_2 = \left(\sum_{i=1}^{n} |y_i - p(t_i)|^2\right)^{1/2},$$

THE LEAST SQUARES PROBLEM

THE DISCRETE LEAST SQUARES PROBLEM

whereas if we choose the 1-norm or the ∞-norm, we minimize respectively the quantities

$$\|r\|_1 = \sum_{i=1}^{n} |y_i - p(t_i)| \qquad \text{and} \qquad \|r\|_\infty = \max_{1\le i\le n} |y_i - p(t_i)|.$$

The problem of finding the minimizing p has been studied for a variety of norms, including those we have just mentioned. By far the nicest theory is that based on the Euclidean norm, and it is that theory that we will study in this chapter. To minimize $\|r\|_2$ is the same as to minimize

$$\|r\|_2^2 = \sum_{i=1}^{n} |y_i - p(t_i)|^2.$$

THE LEAST SQUARES PROBLEM

THE DISCRETE LEAST SQUARES PROBLEM

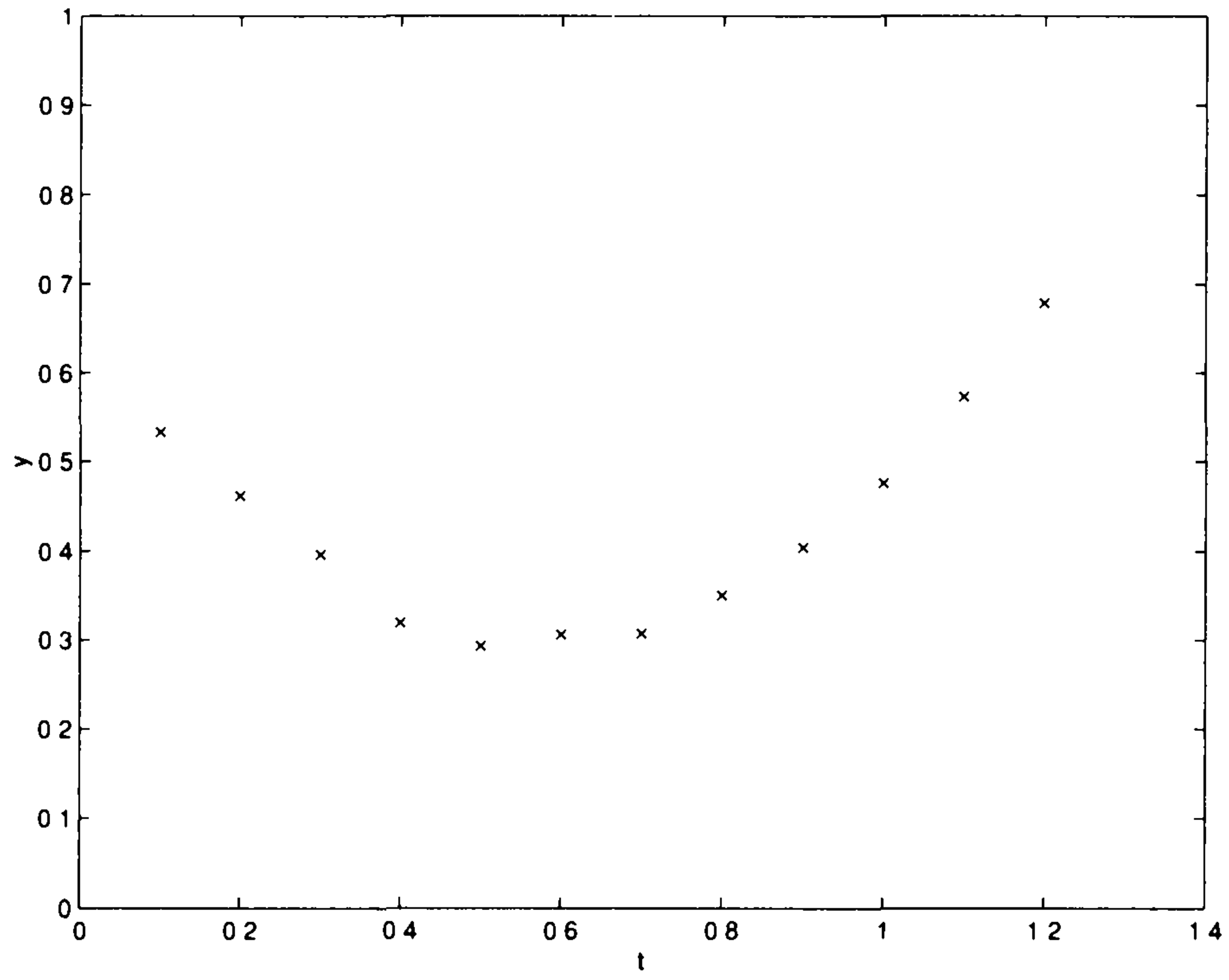
$$\|r\|_2^2 = \sum_{i=1}^{n} |y_i - p(t_i)|^2.$$

Thus we are minimizing the sum of the squares of the residuals. For this reason the problem of minimizing $\|r\|_2$ is called the *least squares problem*.

The choice of the 2-norm can be justified on statistical grounds. Suppose the data fail to lie on a straight line because of errors in the measured y_i. If the errors are independent and normally distributed with mean zero and variance σ^2, then the solution of the least squares problem is the maximum likelihood estimator of the true solution.

THE LEAST SQUARES PROBLEM

THE DISCRETE LEAST SQUARES PROBLEM



Data that can be approximated well by a quadratic polynomial

THE LEAST SQUARES PROBLEM

THE DISCRETE LEAST SQUARES PROBLEM

If we decide to approximate our data by a polynomial of degree $\leq m-1$, then the task is to seek $p(t) = a_0 + a_1 t + a_2 t^2 + \cdots + a_{m-1} t^{m-1}$ such that

$$p(t_i) = y_i \qquad i = 1, \ldots, n. \qquad 1$$

Since the number of data points is typically large and the degree of the polynomial fairly low, it will usually be the case that $n \gg m$. In this case it is too much to ask for a p that satisfies 1 exactly, but for the moment let us act as if that were our goal. The set of polynomials of degree $\leq m-1$ is a vector space of dimension m. If $\phi_1, \phi_2, \ldots, \phi_m$ is a basis of this space, then each polynomial p in the space can be expressed in the form

$$p(t) = \sum_{j=1}^{m} x_j \phi_j(t)$$

THE LEAST SQUARES PROBLEM

THE DISCRETE LEAST SQUARES PROBLEM

$$p(t) = \sum_{j=1}^{m} x_j \phi_j(t) \qquad (3)$$

for some unique choice of coefficients $x_1, x_2, \ldots, x_m$. The obvious basis is $\phi_1(t) = 1$, $\phi_2(t) = t$, $\phi_3(t) = t^2, \ldots, \phi_m(t) = t^{m-1}$, but there are many others, some of which may be better from a computational standpoint. See Example 4.4.15.

Substituting the expression (3) into the equations (1) we obtain a set of n linear equations in the m unknowns $x_1, \ldots, x_m$:

$$\sum_{j=1}^{m} x_j \phi_j(t_i) = y_i, \qquad i = 1, \ldots, n,$$

which can be written in matrix form as

$$\begin{bmatrix} \phi_1(t_1) & \phi_2(t_1) & \cdots & \phi_m(t_1) \\ \phi_1(t_2) & \phi_2(t_2) & \cdots & \phi_m(t_2) \\ \phi_1(t_3) & \phi_2(t_3) & \cdots & \phi_m(t_3) \\ \vdots & \vdots & & \vdots \\ \phi_1(t_n) & \phi_2(t_n) & \cdots & \phi_m(t_n) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix}. \qquad (4)$$

THE LEAST SQUARES PROBLEM

THE DISCRETE LEAST SQUARES PROBLEM

$$\begin{bmatrix} \phi_1(t_1) & \phi_2(t_1) & \cdots & \phi_m(t_1) \\ \phi_1(t_2) & \phi_2(t_2) & \cdots & \phi_m(t_2) \\ \phi_1(t_3) & \phi_2(t_3) & \cdots & \phi_m(t_3) \\ \vdots & \vdots & & \vdots \\ \phi_1(t_n) & \phi_2(t_n) & \cdots & \phi_m(t_n) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix}.$$

If $n > m$, as is usually the case, this is an *overdetermined system*; that is, it has more equations than unknowns. Thus we cannot expect to find an x that satisfies 1 exactly. Instead we might seek an x for which the sum of the squares of the residuals is minimized.

THE LEAST SQUARES PROBLEM

THE DISCRETE LEAST SQUARES PROBLEM

It is easy to imagine further generalizations of this problem. For example, the functions $\phi_1, \ldots, \phi_m$ could be taken to be trigonometric or exponential or some other kind of functions. More generally we can consider the overdetermined system

$$Ax = b,$$

$A \in \mathbb{R}^{n \times m}, \; n > m, b \in \mathbb{R}^n$

Least squares problem

Find x $\min_{x \in \mathbb{R}^m} \|b - Ax\|_2$

($r = b - Ax$) is the residual.

THE LEAST SQUARES PROBLEM

Exercise 1 Consider the following data.

t_i	1.0	1.5	2.0	2.5	3.0
y_i	1.1	1.2	1.3	1.3	1.4

Julia

(a) Set up an overdetermined system of the form 4 for a straight line passing through the data points. Use the standard basis polynomials $\phi_1(t) = 1$, $\phi_2(t) = t$.

(b) Use Julia to calculate the least-squares solution of the system from part (a). This is a simple matter. Given an overdetermined system $Ax = b$, the Julia command `x = A\b` computes the least squares solution. Recall that this is exactly the same command as would be used to tell Julia to solve a square system $Ax = b$ by Gaussian elimination.[16] Some useful Julia commands:

```
t = 1:.5:3; t = t'; s = ones(5,1); A = [s t];
```

THE LEAST SQUARES PROBLEM

Exercise 1 continued

We already know that Julia uses Gaussian elimination with partial pivoting in the square case. In the next two sections you will find out what Julia does in the overdetermined case.

(c) Use the Julia `plot` command to plot the five data points and your least squares straight line. Type ? `plot` for information about using the plot command, or search in Julia's help browser.

(d) Use Julia to compute $\| r \|_2$, the norm of the residual.

THE LEAST SQUARES PROBLEM

ORTHOGONAL MATRICES, ROTATORS, AND REFLECTORS

We begin by introducing an inner product in $\mathbb{R}^n$. Given two vectors $x = [x_1, \ldots, x_n]^T$ and $y = [y_1, \ldots, y_n]^T$ in $\mathbb{R}^n$, we define the *inner product* of x and y, denoted $\langle x, y \rangle$ by

$$\langle x, y \rangle = \sum_{i=1}^{n} x_i y_i .$$

Although the inner product is a real number, it can also be expressed as a matrix product:

$$\langle x, y \rangle = y^T x = x^T y.$$

The inner product has the following properties, which you can easily verify:

$$\begin{aligned}
\langle x, y \rangle &= \langle y, x \rangle \\
\langle \alpha_1 x_1 + \alpha_2 x_2, y \rangle &= \alpha_1 \langle x_1, y \rangle + \alpha_2 \langle x_2, y \rangle \\
\langle x, \alpha_1 y_1 + \alpha_2 y_2 \rangle &= \alpha_1 \langle x, y_1 \rangle + \alpha_2 \langle x, y_2 \rangle \\
\langle x, x \rangle &\geq 0 \qquad \text{with equality if and only if } x = 0.
\end{aligned}$$

THE LEAST SQUARES PROBLEM

ORTHOGONAL MATRICES, ROTATORS, AND REFLECTORS

Note also the close relationship between the inner product and the Euclidean norm:

$$\| x \|_2 = \sqrt{\langle x, x \rangle}.$$

The Cauchy-Schwarz inequality (See part 1) can be stated more concisely in terms of the inner product and the Euclidean norm: For every x, $y \in \mathbb{R}^n$,

$$|\langle x, y \rangle| \le \| x \|_2 \| y \|_2.$$

5

When $n = 2$ (or 3) the inner product coincides with the familiar dot product from analytic geometry. Recall that if x and y are two nonzero vectors in a plane and θ is the angle between them, then

$$\cos\theta = \frac{\langle x, y \rangle}{\| x \|_2 \| y \|_2}.$$

THE LEAST SQUARES PROBLEM

ORTHOGONAL MATRICES, ROTATORS, AND REFLECTORS

Orthogonal Matrices

A matrix $Q \in \mathbb{R}^{n \times n}$ is said to be *orthogonal* if $QQ^T = I$. This equation says that Q has an inverse, and $Q^{-1} = Q^T$. Since a matrix always commutes with its inverse, we have $Q^T Q = I$ as well. For square matrices the equations

$$QQ^T = I \qquad Q^T Q = I \qquad Q^T = Q^{-1}$$

are all equivalent, and any one of them could be taken as the definition of an orthogonal matrix.

Exercise 2 (a) Show that if Q is orthogonal, then Q^{-1} is orthogonal. (b) Show that if Q_1 and Q_2 are orthogonal, then $Q_1 Q_2$ is orthogonal. $\square$

Exercise 3 Show that if Q is orthogonal, then $\det(Q) = \pm 1$.

Theorem 1 *If $Q \in \mathbb{R}^{n \times n}$ is orthogonal, then for all x, $y \in \mathbb{R}^n$,*

$$(a)\ \langle Qx, Qy \rangle = \langle x, y \rangle, \qquad (b)\ \| Qx \|_2 = \| x \|_2.$$

Proof. (a) $\langle Qx, Qy \rangle = (Qy)^T(Qx) = y^T Q^T Qx = y^T I x = y^T x = \langle x, y \rangle$.
(b) Set $y = x$ in part (a) and take square roots.

Part (b) of the theorem says that Qx and x have the same length. Thus *orthogonal transformations preserve lengths*. Combining parts (a) and (b), we see that

$$\arccos \frac{\langle Qx, Qy \rangle}{\| Qx \|_2 \| Qy \|_2} = \arccos \frac{\langle x, y \rangle}{\| x \|_2 \| y \|_2}.$$

Thus the angle between Qx and Qy is the same as the angle between x and y. We conclude that *orthogonal transformations preserve angles*.

THE LEAST SQUARES PROBLEM

ORTHOGONAL MATRICES, ROTATORS, AND REFLECTORS

When using part (b) of theorem 1 in the least squares problem we can see that for every orthogonal Q we have

$$\| b - Ax \|_2 = \| Qb - QAx \|_2 .$$

We can see that the solution of least squares is unchanged if we replace by Qb and Ax by QAx.

We can then find Q such that QA is very simple

THE LEAST SQUARES PROBLEM

ORTHOGONAL MATRICES, ROTATORS, AND REFLECTORS

Exercise 4 Show that if Q is orthogonal, then $\| Q \|_2 = 1$, $\| Q^{-1} \|_2 = 1$, and $\kappa_2(Q) = 1$. thus Q is perfectly conditioned with respect to the 2-condition number. This suggests that orthogonal matrices will have good computational properties. □

There are 2 two types of orthogonal transformations that are widely used in matrix computation: **rotators** (**Givens Transformation**) and **reflectors (Householder Transformation)**

Together with the Gaussian elimination, these are fundamental building blocks of matrix computation

THE LEAST SQUARES PROBLEM

ORTHOGONAL MATRICES, ROTATORS, AND REFLECTORS

Rotators

Consider vectors in the plane $\mathbb{R}^2$. The operator that rotates each vector through a fixed angle θ is a linear transformation, so it can be represented by a matrix. Let

$$Q = \begin{bmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \end{bmatrix}$$

be this matrix. Then Q is completely determined by its action on the two vectors $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$, because

$$\begin{bmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} q_{11} \\ q_{21} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} q_{12} \\ q_{22} \end{bmatrix}.$$

THE LEAST SQUARES PROBLEM

ORTHOGONAL MATRICES, ROTATORS, AND REFLECTORS

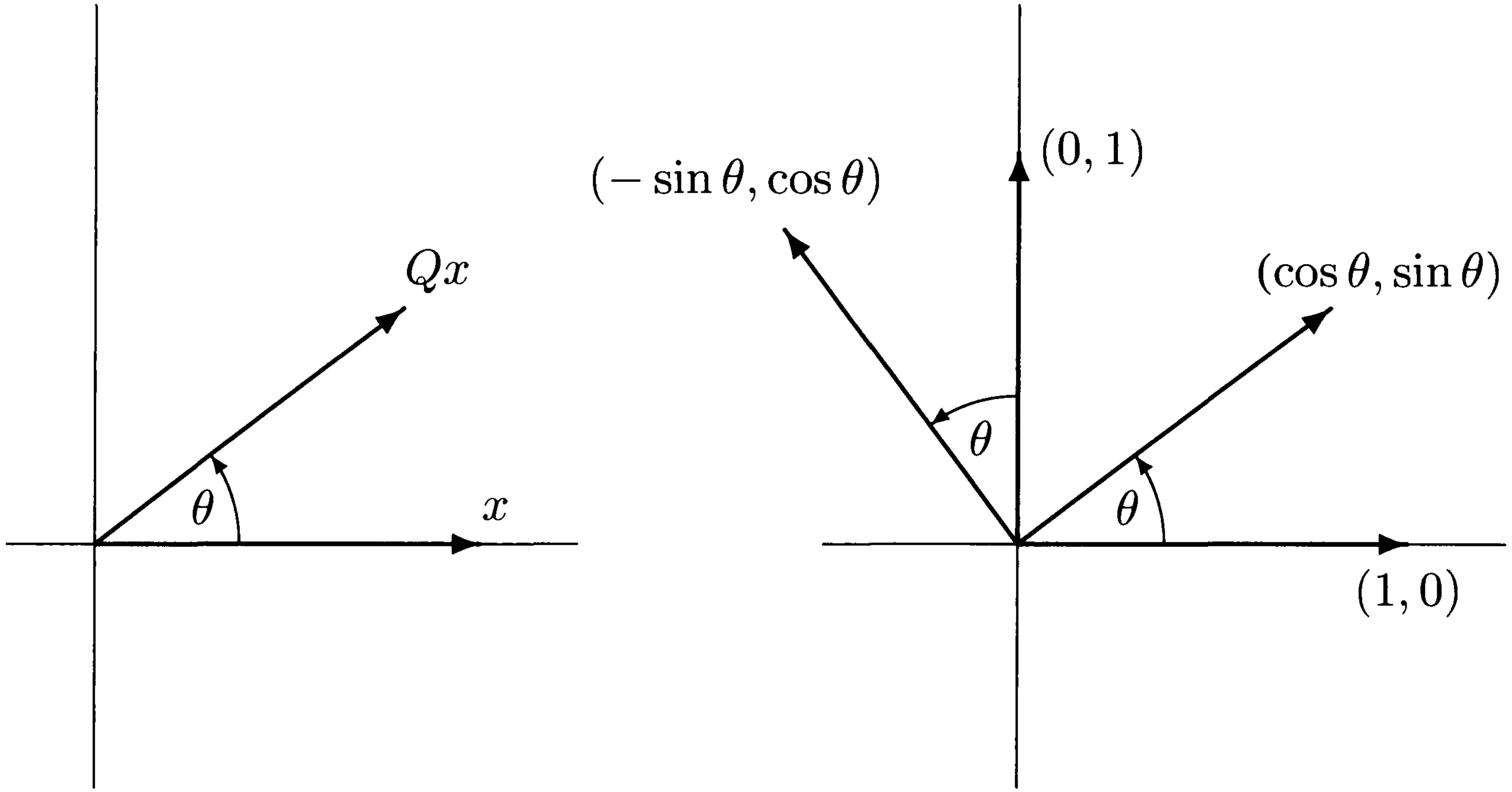


Figure 1

THE LEAST SQUARES PROBLEM

ORTHOGONAL MATRICES, ROTATORS, AND REFLECTORS

Since the action of Q is to rotate each vector through the angle θ, clearly (see Figure 1)

$$Q\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix} \quad \text{and} \quad Q\begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} -\sin\theta \\ \cos\theta \end{bmatrix}.$$

Thus $\begin{bmatrix} q_{11} \\ q_{21} \end{bmatrix} = \begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix}$ and $\begin{bmatrix} q_{12} \\ q_{22} \end{bmatrix} = \begin{bmatrix} -\sin\theta \\ \cos\theta \end{bmatrix}$; that is,

$$Q = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}.$$

A matrix of this form is called a *rotator* or *rotation*.

THE LEAST SQUARES PROBLEM

ORTHOGONAL MATRICES, ROTATORS, AND REFLECTORS

Exercise 5 Verify that every rotator is an orthogonal matrix with determinant 1. What does the inverse of a rotator look like? What transformation does it represent? □

Rotators can be used to create zeros in a vector or matrix. For example, if $x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ is a vector with $x_2 \neq 0$, let us see how to find a rotator

$$Q = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

such that $Q^T x$ has a zero in its second component: $Q^T x = \begin{bmatrix} y \\ 0 \end{bmatrix}$ for some y. Now

$$Q^T x = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} (\cos\theta)x_1 + (\sin\theta)x_2 \\ -(\sin\theta)x_1 + (\cos\theta)x_2 \end{bmatrix},$$

which has the form $\begin{bmatrix} y \\ 0 \end{bmatrix}$ if and only if

$$x_1 \sin\theta = x_2 \cos\theta. \qquad 6$$

THE LEAST SQUARES PROBLEM

ORTHOGONAL MATRICES, ROTATORS, AND REFLECTORS

Thus θ can be taken to be $\arctan(x_2/x_1)$ or any other angle satisfying $\tan\theta = x_2/x_1$.

Clearly $\cos\theta = x_1$ and $\sin\theta = x_2$ satisfy 6

We can determine without determine θ itself.

We can take $$\cos\theta = \frac{x_1}{\sqrt{x_1^2 + x_2^2}} \quad \text{and} \quad \sin\theta = \frac{x_2}{\sqrt{x_1^2 + x_2^2}},$$

Such that $\cos^2\theta + \sin^2\theta = 1$

THE LEAST SQUARES PROBLEM

ORTHOGONAL MATRICES, ROTATORS, AND REFLECTORS

Now let us see how we can use a rotator to simplify a matrix

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}.$$

We have seen that there is a rotator Q such that

$$Q^T \begin{bmatrix} a_{11} \\ a_{21} \end{bmatrix} = \begin{bmatrix} r_{11} \\ 0 \end{bmatrix}, \qquad \text{where } r_{11} = \sqrt{a_{11}^2 + a_{21}^2}.$$

Defined r_{12} and r_{22} by $$\begin{bmatrix} r_{12} \\ r_{22} \end{bmatrix} = Q^T \begin{bmatrix} a_{12} \\ a_{22} \end{bmatrix},$$

and let

$$R = \begin{bmatrix} r_{11} & r_{12} \\ 0 & r_{22} \end{bmatrix}.$$

THE LEAST SQUARES PROBLEM

ORTHOGONAL MATRICES, ROTATORS, AND REFLECTORS

Then $Q^T A = R$. This shows that we can transform A to an upper triangular matrix by multiplying it by the orthogonal matrix Q^T. As we shall soon see, it is possible to carry out such a transformation not just for 2-by-2 matrices, but for all $A \in \mathbb{R}^{n \times n}$.

That is, for every $A \in \mathbb{R}^{n \times n}$ there is an orthogonal matrix $Q \in \mathbb{R}^{n \times n}$ and an upper triangular matrix $R \in \mathbb{R}^{n \times n}$ such that $Q^T A = R$.

We can use this transformation to solve the linear system $Ax = b$.

Multiplying the left and right hand sides by Q^T, we have $Q^T Ax = Q^T b = c$

Let $R = Q^T A$ then we solve the upper triangular system $Rx = c$, by substitution.