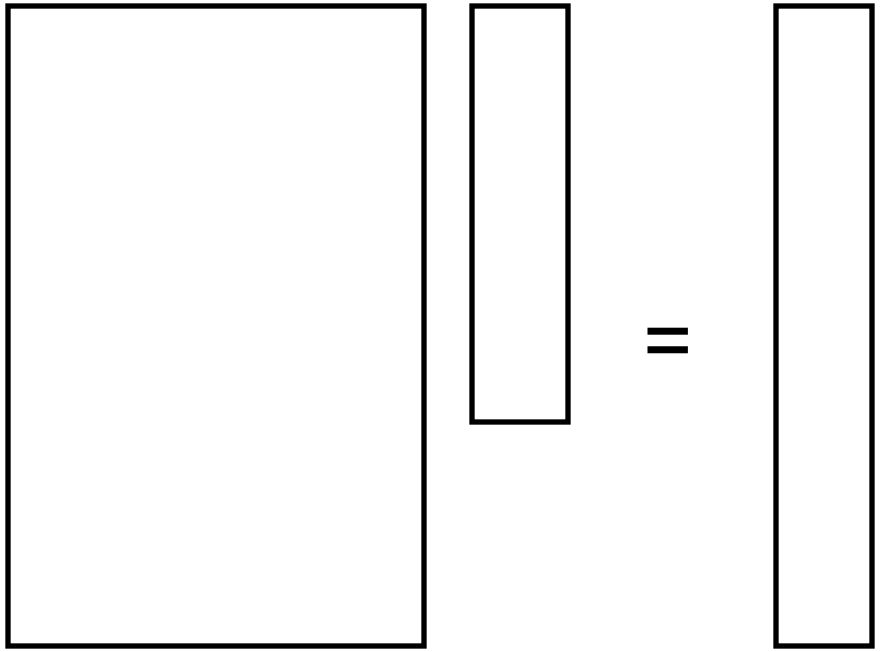
GEO 242: Numerical methods and modeling in the geosciences



A x = b

Outline

Simultaneous equations

A x = **b** for non-square matrices

The least squares problem

Where this is heading…

The lectures in the rest of the quarter will cover some very simple concepts related to simple modeling of data (e.g. curve fitting, function fitting). There will be some math, but really only enough to show you the point.

Specifically, we are going to look at the relationship between model parameters (the inputs to a model) and data

Forward and inverse models

Forward models are models where we know the parameters, and also the theory relating them to observations, and we want to make predictions of the effects

Inverse models are models where we know the theory, and have observations, and we want to infer the parameters

Most of the time, we are working with inverse modeling problems…

Linear and nonlinear models

Linear models are models where the calculations of predicted observations (**d**) are a product between the theory (**A**) and the model parameters (**m**), i.e.

$$\mathbf{A}\,\mathbf{m} = \mathbf{d}$$

Nonlinear models are those where the model calculation is a function of the model parameters, but not a product, i.e.

$$\mathbf{d} = \mathbf{A}(\mathbf{m})$$

We will cover both types in the class, starting with the linear models, since they are easier!

Simultaneous equations

An example of a pair of simultaneous equations…

$$x + 2y = 4 \qquad (1)$$

$$x - y = 1 \qquad (2)$$

To solve:

i) Multiply (2) by 2

ii) Add to (1)

iii) Solve for x

iv) Plug value of x into (2) and solve for y

A matrix representation

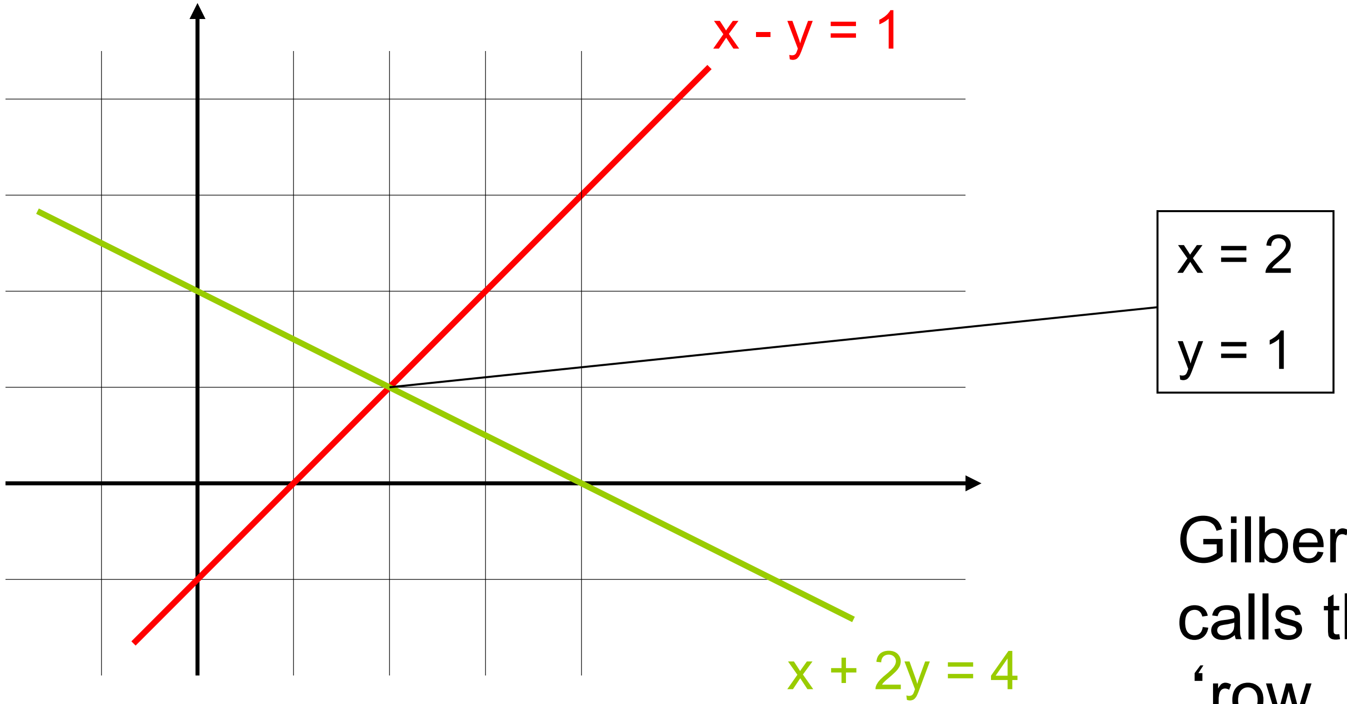
The same pair of equations can be represented in matrix form:

$$\begin{bmatrix} 1 & 2 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 4 \\ 1 \end{bmatrix}$$

A x = b

A graphical representation

When we solve a pair of simultaneous equations, we are effectively finding the point where the two lines defined by the equations intersect



Gilbert Strang calls this the 'row representation'

The 'column' representation

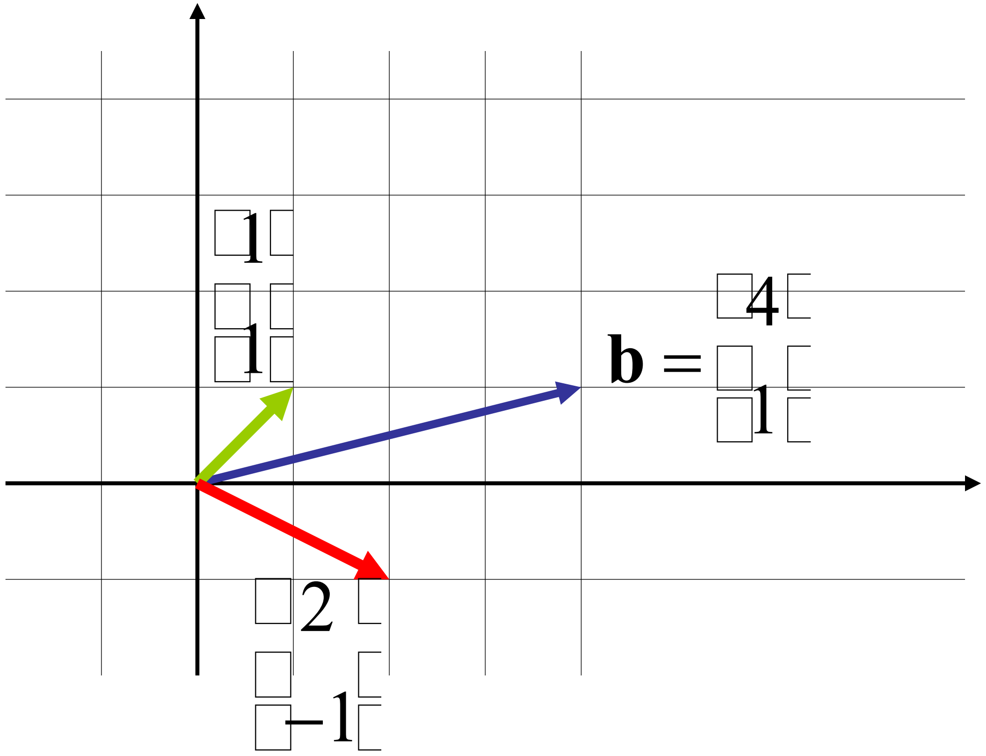
Instead of plotting the lines, we can divide up the x and y components of the two equations like so:

$$x\begin{bmatrix}1\\1\end{bmatrix}+y\begin{bmatrix}2\\-1\end{bmatrix}=\begin{bmatrix}4\\1\end{bmatrix}$$

In this case, we see the correct *linear combination* of the two column vectors on the left hand side to give the vector **b**.

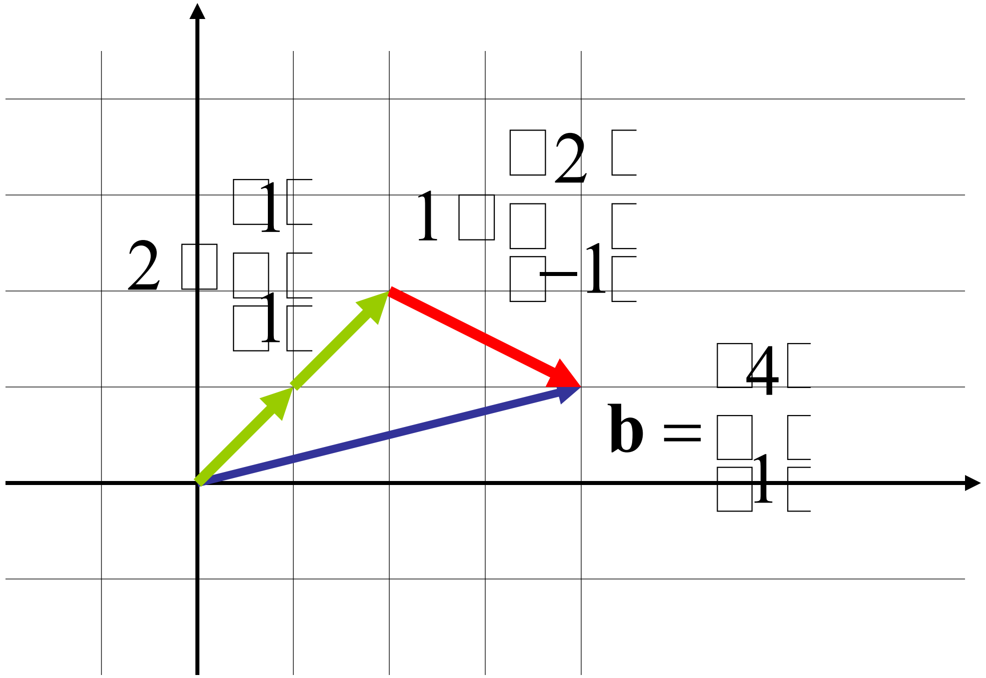
A graphical representation

In the column representation, we seek the correct linear combination of column vectors to give us **b**



A graphical representation

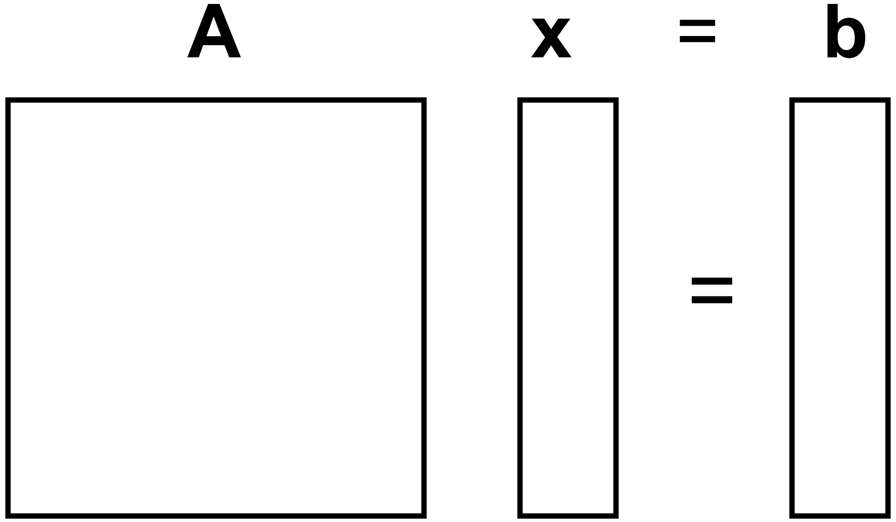
In the column representation, we seek the correct linear combination of column vectors to give us **b**



$$x\begin{bmatrix}1\\1\end{bmatrix}+y\begin{bmatrix}2\\-1\end{bmatrix}=\begin{bmatrix}4\\1\end{bmatrix}$$

$$(2)\begin{bmatrix}1\\1\end{bmatrix}+(1)\begin{bmatrix}2\\-1\end{bmatrix}=\begin{bmatrix}4\\1\end{bmatrix}$$

A well-posed problem



If the columns of **A** are independent, then some linear combination of them will match the vector **b**. This is a unique solution! We would say such a problem is 'well posed'.

The inverse of a matrix

The inverse of a square matrix, **A**, is defined as the matrix that, when **A** is multiplied by it, the product is an identity matrix, **I**, i.e.

$$\mathbf{A}\,\mathbf{A}^{-1} = \mathbf{A}^{-1}\,\mathbf{A} = \mathbf{I}$$

If the inverse is known, it can be used to solve the **A x = b** problem:

$$\mathbf{A}^{-1}\,\mathbf{A}\,\mathbf{x} = \mathbf{A}^{-1}\,\mathbf{b}$$

$$\mathbf{I}\,\mathbf{x} = \mathbf{A}^{-1}\,\mathbf{b}$$

$$\mathbf{x} = \mathbf{A}^{-1}\,\mathbf{b}$$

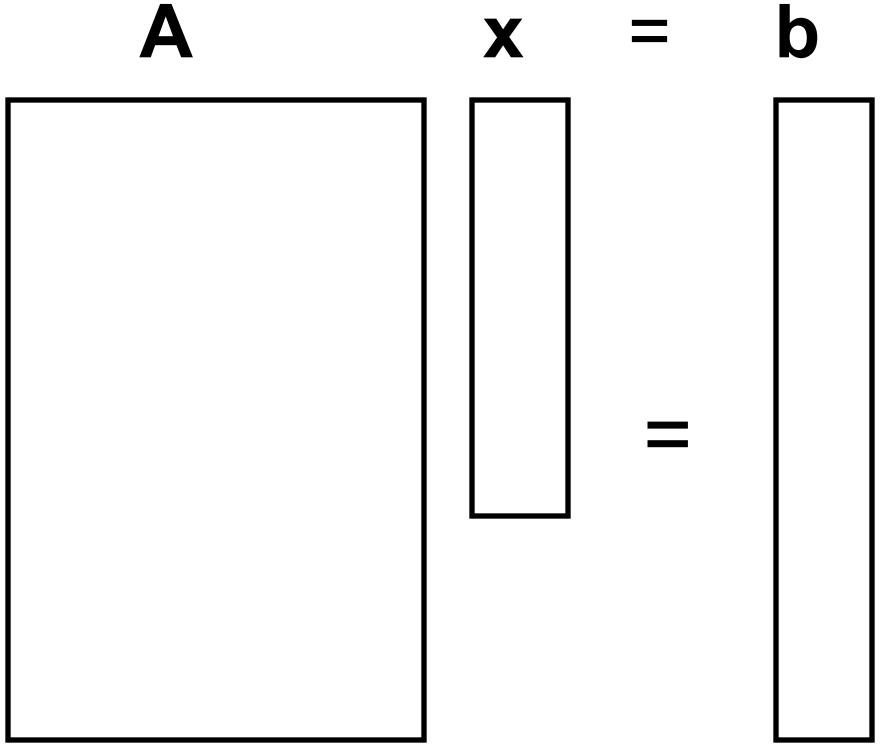
'Real' linear systems

In reality, linear systems are often not 'well-posed' (i.e. with as many unknowns as equations)

All of the cases we have considered thus far have been square matrices, where the number of independent rows was the same as the number of rows (or else, they were singular)

What do we do with 'real' systems?

Dense linear algebra



A x = **b** (and its relatives) is the standard equation for linear systems

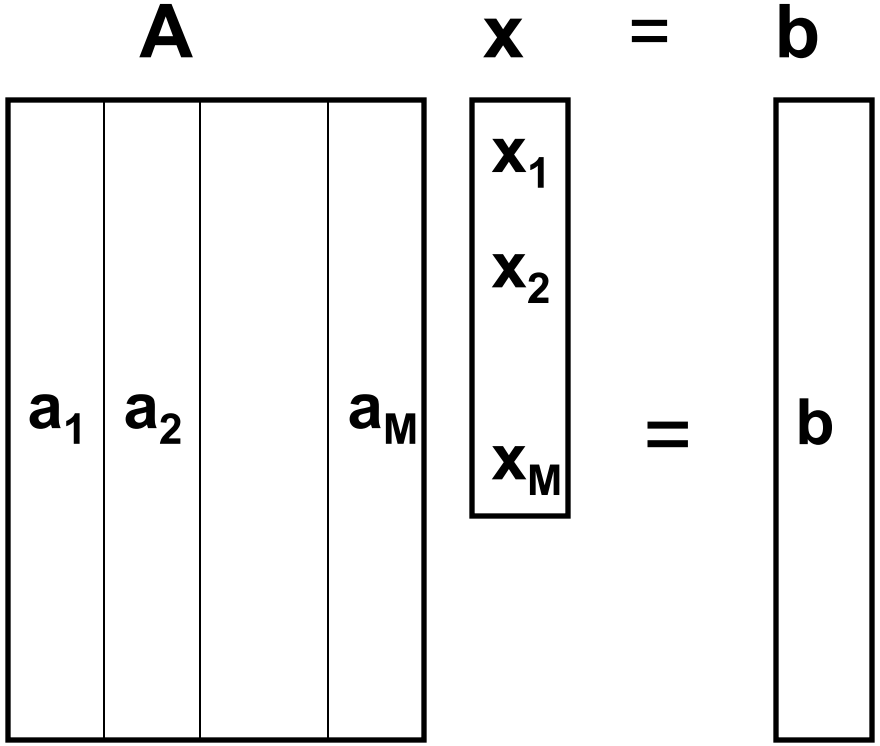
Forward and inverse models

If you have a *design matrix* **A** that incorporates some physical theory, with **x** representing the values of model parameters

A x will provide a *forward model* of the data **b**, without necessarily knowing what the correct values of **b** or **x** are

In contrast, if the data **b** are known, then by inverting matrix **A** we can attempt an *inverse model*, where the values of the model parameters are those such that the values of **A x** – **b** (the ‘residuals’) are small

Dense linear algebra



b is a linear combination of the column vectors in **A**, i.e. $\mathbf{b} = \sum_{j=1}^{M} x_j \mathbf{a}_j$

Rank deficiency

The 'range' of a matrix (which we are treating here as a set of columns, or a 'column space') is the set of all such linear combinations

The range of **A** in this case is thus a 'vector space' with a dimension ≤ M

This dimension is given by the rank of **A**

If rank(**A**) < M, then **A** is said to be 'rank deficient'; if rank(**A**) = M, then **A** is 'full rank', of course

$\mathbf{A}\ \mathbf{x} = \mathbf{b}$ or $\mathbf{A}\ \mathbf{x} \approx \mathbf{b}$?

One thing we might wonder is whether there exists a vector $\mathbf{x}$ such that $\mathbf{A}\ \mathbf{x}$ is exactly equal to $\mathbf{b}$

Let's suppose that $\mathbf{A}$ is square and full rank:

In that case, $\mathbf{A}\ \mathbf{x} = \mathbf{b}$ has a unique solution for each $\mathbf{b}$, given by $\mathbf{x} = \mathbf{A}^{-1}\ \mathbf{b}$

What if $\mathbf{A}$ is rectangular?

Well, then unless $\mathbf{b} \in \mathrm{range}(\mathbf{A})$, $\mathbf{A}\ \mathbf{x} = \mathbf{b}$ has no exact solution

[$\in$ = 'is a member of']

$\mathbf{A}\ \mathbf{x} = \mathbf{b}$ or $\mathbf{A}\ \mathbf{x} \approx \mathbf{b}$?

Even if there is no exact solution, we may be able to find one that is close, i.e. find $\mathbf{x}$ such that $\mathbf{A}\ \mathbf{x} \approx \mathbf{b}$

This is the underlying concept of the method of least squares…

Least squares problems

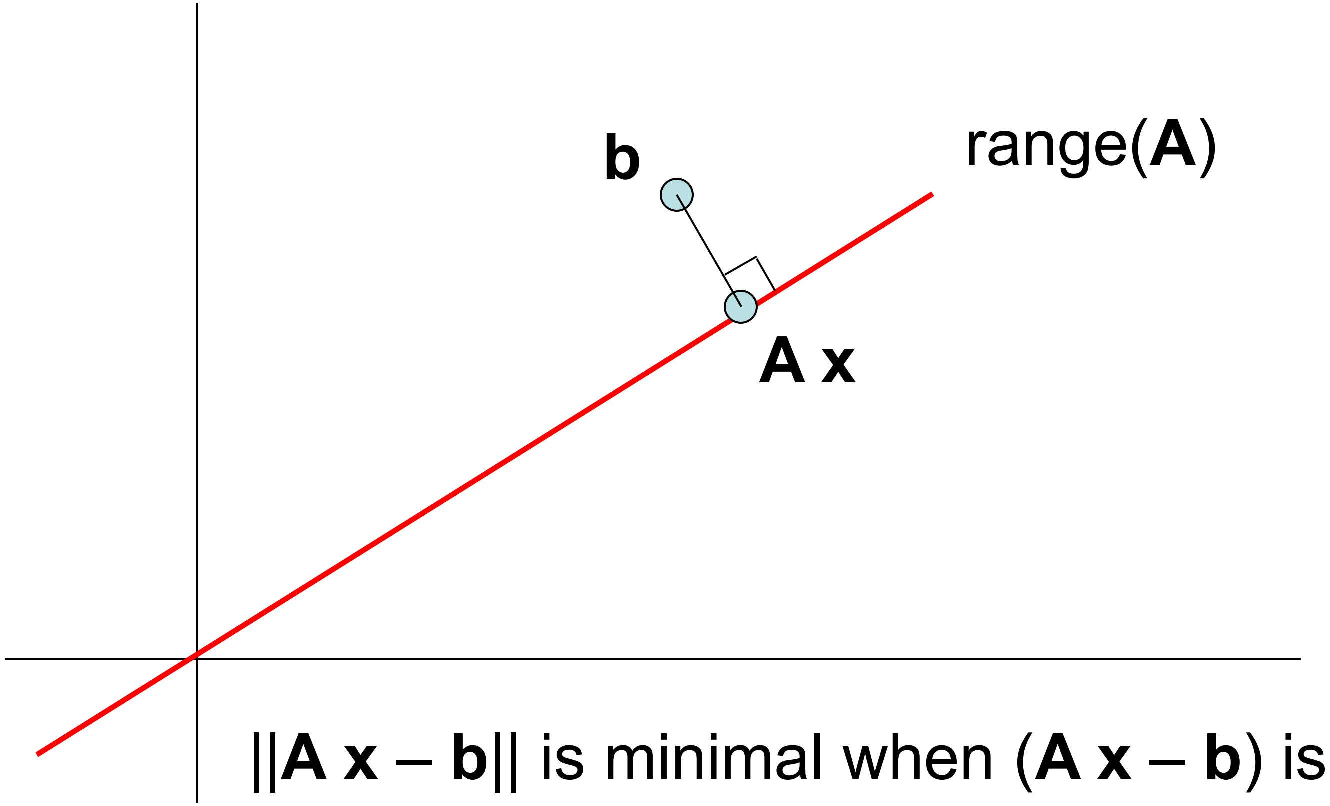
We define the 2-norm (root squared sum) of a vector, **v**, to be

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

The least squares solution to an inverse problem, **A x** = **b**, is a vector **x**, such that ||**A x** – **b**|| = minimal

Least squares problems

In graphical form:



||**A x** – **b**|| is minimal when (**A x** – **b**) is orthogonal to range(**A**)

Least squares problems

We seek the vector **x** such that (**A x** – **b**) is perpendicular to range(**A**)

[range(**A**), remember, is the space of linear combinations of $\mathbf{a}_j$, the columns of **A**]

i.e.

$$\mathbf{b} - \mathbf{A}\mathbf{x} \perp \mathrm{range}(\mathbf{A})$$

$$\Leftrightarrow \mathbf{b} - \mathbf{A}\mathbf{x} \perp \mathbf{a}_j$$

$$\Leftrightarrow \mathbf{a}_j^{T}(\mathbf{b} - \mathbf{A}\mathbf{x}) = 0$$

$$\Leftrightarrow \mathbf{A}^{T}(\mathbf{b} - \mathbf{A}\mathbf{x}) = 0$$

Least squares problems

$$\Leftrightarrow \mathbf{A}^T(\mathbf{b} - \mathbf{A}\mathbf{x}) = 0$$

$$\Leftrightarrow \mathbf{A}^T\mathbf{b} - \mathbf{A}^T\mathbf{A}\mathbf{x} = 0$$

$$\Leftrightarrow \boxed{\mathbf{A}^T\mathbf{A}\mathbf{x} = \mathbf{A}^T\mathbf{b}}$$

This matrix equation represents a system of linear equations known as the *normal equations*, so-called because the solution **x**, gives the vector (**A x** – **b**) that is normal to the range of **A**

Least squares problems

$$\Leftrightarrow \mathbf{A}^{\mathrm{T}}(\mathbf{b} - \mathbf{A}\mathbf{x}) = 0$$

$$\Leftrightarrow \mathbf{A}^{\mathrm{T}}\mathbf{b} - \mathbf{A}^{\mathrm{T}}\mathbf{A}\mathbf{x} = 0$$

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This matrix equation represents a system of linear equations known as the *normal equations*, so-called because the solution **x**, gives the vector (**A x** – **b**) that is normal to the range of **A**

As a bonus, the matrix $\mathbf{A}^{\mathrm{T}}\mathbf{A}$ is square, and can easily be inverted (NB if well posed)

Least squares problems

How can we pose line-fitting as a matrix problem? And how, then can we solve it using the least squares method?

The CO_2 record at Mauna Loa

The 'Keeling Curve', based on the record of atmospheric CO_2 as measured at the Scripps Mauna Loa Observatory, is one of the most famous such records in the world. Let's estimate the trend!

1) Find, and get the monthly records from Mauna Loa
2) Parse the data and get them into a format suitable to read into Python, load them in and plot them
3) Set up and solve the inverse problem to fit a straight line to the data, and plot the agreement
4) Try to fit some other functions (quadratic, cubic, quartic, quintic) and evaluate them all to project CO_2 emissions out to 2100