Linear Algebra for Machine Learning in Python

Moritz Wolter

September 13, 2022

High Performance Computing and Analytics Lab, University of Bonn

Overview

Introduction

Essential operations

Linear curve fitting

Regularization

Introduction

Motivating linear algebra

Même le feu est régi par les nombres.

Fourier[1] studied the transmission of heat using tools that would later be called an eigenvector-basis. Why would he say something like this?

[1] Jean Baptiste Joseph Fourier (1768-1830)

Matrices

$\mathbf{A} \in \mathbb{R}^{m,n}$ is a real-valued Matrix with m rows and n columns.

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{pmatrix}, a_{ij} \in \mathbb{R}. \tag{1}$$

Essential operations

Addition

To matrices $\mathbf{A} \in \mathbf{R}^{m,n}$ and $\mathbf{B} \in \mathbf{R}^{m,n}$ can be added by adding their elements.

$$\mathbf{A} + \mathbf{B} = \begin{pmatrix} a_{11} + b_{11} & a_{12} + b_{12} & \dots & a_{1n} + b_{1n} \\ a_{21} + b_{21} & a_{22} + b_{22} & \dots & a_{2n} + b_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} + b_{m1} & a_{m2} + b_{m2} & \dots & a_{mn} + b_{mn} \end{pmatrix} \tag{2}$$

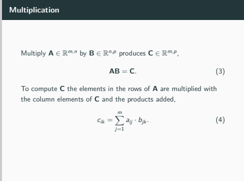
Multiplication

Multiply $\mathbf{A} \in \mathbb{R}^{m,n}$ by $\mathbf{B} \in \mathbb{R}^{n,p}$ produces $\mathbf{C} \in \mathbb{R}^{m,p}$,

$$\mathbf{AB} = \mathbf{C}. \tag{3}$$

To compute $\mathbf{C}$ the elements in the rows of $\mathbf{A}$ are multiplied with the column elements of $\mathbf{C}$ and the products added,

$$c_{ik} = \sum_{j=1}^{m} a_{ij} \cdot b_{jk}. \tag{4}$$



Define on the board:

- Dot product $\mathbf{a} \cdot \mathbf{b} = a_1 b_1 + a_2 b_2 + \cdots + a_n b_n$ for two vectors $\mathbf{a}, \mathbf{b} \in \mathbb{R}^n$.
- Row times column view [Str+09]:

The identity matrix

$$\mathbf{I} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{pmatrix} \tag{5}$$

The identity matrix

$$\mathbf{I} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{pmatrix} \tag{5}$$

Demonstrate multiplication with the inverse by hand.

$$\begin{pmatrix} -1 & 0 & 0 \\ 1 & -1 & 1 \\ 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} -1 & -0 & -0 \\ -2 & -1 & -1 \\ -1 & -0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{6}$$

Matrix inverse

The inverse Matrix $\mathbf{A}^{-1}$ undoes the effects of $\mathbf{A}$, or in mathematical notation,

$$\mathbf{A}\mathbf{A}^{-1} = \mathbf{I}. \tag{7}$$

The process of computing the inverse is called Gaussian elimination.

Matrix inverse

The inverse Matrix $\mathbf{A}^{-1}$ undoes the effects of $\mathbf{A}$, or in mathematical notation,

$$\mathbf{A}\mathbf{A}^{-1} = \mathbf{I}. \tag{7}$$

The process of computing the inverse is called Gaussian elimination.

Example on the board:

$$\mathbf{A} = \begin{pmatrix} 2 & 0 \\ 1 & 3 \end{pmatrix} \rightsquigarrow \left(\begin{array}{cc|cc} 2 & 0 & 1 & 0 \\ 1 & 3 & 0 & 1 \end{array}\right) \rightsquigarrow \left(\begin{array}{cc|cc} 1 & 0 & \frac{1}{2} & 0 \\ 1 & 3 & 0 & 1 \end{array}\right) \tag{8}$$

$$\rightsquigarrow \left(\begin{array}{cc|cc} 1 & 0 & \frac{1}{2} & 0 \\ 0 & 3 & -\frac{1}{2} & 1 \end{array}\right) \rightsquigarrow \left(\begin{array}{cc|cc} 1 & 0 & \frac{1}{2} & 0 \\ 0 & 1 & -\frac{1}{6} & \frac{1}{3} \end{array}\right) \tag{9}$$

Test the result:

$$\begin{pmatrix} 2 & 0 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & 0 \\ -\frac{1}{6} & \frac{1}{3} \end{pmatrix} = \begin{pmatrix} 2 \cdot \frac{1}{2} + 0 \cdot -\frac{1}{6} & 2 \cdot 0 + 0 \cdot \frac{1}{3} \\ 1 \cdot \frac{1}{2} + 3 \cdot -\frac{1}{6} & 0 \cdot 0 + 3 \cdot \frac{1}{3} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{10}$$

The Transpose

The transpose operation flips matrices along the diagonal, for example, in $\mathbb{R}^2$,

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^T = \begin{pmatrix} a & c \\ b & d \end{pmatrix} \tag{11}$$

Motivation of the determinant

- The determinant contains lots of information about a matrix in a single number.
- When a Matrix has a zero determinant, it's inverse does not exist.

Computing determinants in two or three dimensions

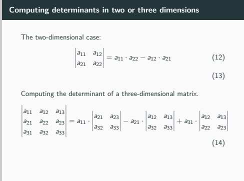
The two-dimensional case:

$$\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11} \cdot a_{22} - a_{12} \cdot a_{21} \tag{12}$$

$$\tag{13}$$

Computing the determinant of a three-dimensional matrix.

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = a_{11} \cdot \begin{vmatrix} a_{21} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} - a_{21} \cdot \begin{vmatrix} a_{12} & a_{13} \\ a_{32} & a_{33} \end{vmatrix} + a_{31} \cdot \begin{vmatrix} a_{12} & a_{13} \\ a_{22} & a_{23} \end{vmatrix} \tag{14}$$



Draw the sign pattern on the board:

$$\begin{vmatrix} + & - & + & \dots \\ - & + & - & \dots \\ + & - & + & \dots \\ \vdots & \vdots & \vdots & \ddots \end{vmatrix} \tag{15}$$

The determinant can be expanded along any column as long as the sign pattern is respected.

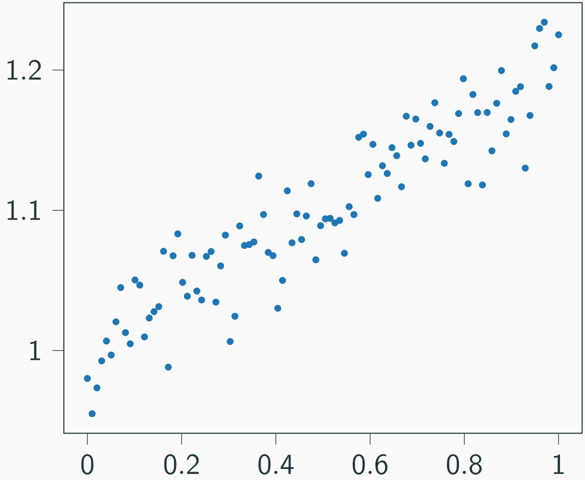
Determinants in n-dimensions

$$\begin{vmatrix} a_{11} & a_{21} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{vmatrix} = a_{11} \begin{vmatrix} a_{22} & \dots & a_{2n} \\ \vdots & & \vdots \\ a_{m2} & \dots & a_{mn} \end{vmatrix} + a_{21} \begin{vmatrix} a_{21} & \dots & a_{2n} \\ \vdots & & \vdots \\ a_{m2} & \dots & a_{mn} \end{vmatrix}$$

$$-a_{m1} \begin{vmatrix} a_{11} & \dots & a_{1n} \\ a_{21} & \dots & a_{2n} \\ \vdots & & \vdots \end{vmatrix}$$

Linear curve fitting

What is the best line connecting measurements?



Problem Formulation

A line has the form $cx + d$, with $c, x, d \in \mathbb{R}$. In matrix language we could ask for every point to be on the line,

$$\begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix} \begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} p_1 \\ p_2 \\ \vdots \\ p_n \end{pmatrix}. \tag{16}$$

We can treat polynomials as vectors, too! The coordinates populate the matrix rows in $\mathbf{A} \in \mathbb{R}^{n_p \times 2}$, and the coefficients appear in $\mathbf{x} \in \mathbb{R}^2$, with the points we would like to model in $\mathbf{b} \in \mathbb{R}^{n_p}$. The problem now appears in matrix form and can be solved using linear algebra!

The Pseudoinverse [Str+09; DFO20]

The inverse we saw earlier only exsits for sqaure that is n by n matrices. Nonsqaure $\mathbf{A}$ such as the one we just saw, require the pseudoinverse,

$$\mathbf{A}^{\dagger} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T. \tag{17}$$

Sometimes solving $\mathbf{Ax} + \mathbf{b} = 0$ is implossible, the pseudoinverse considers,

$$\min_x \frac{1}{2}|\mathbf{Ax} - \mathbf{b}|^2 \tag{18}$$

$$\tag{19}$$

instead. $\mathbf{A}^{\dagger}\mathbf{b} = \mathbf{x}$ yields the solution.

The Pseudoinverse [Str+09; DFO20]

The inverse we saw earlier only exsits for sqaure that is n by n matrices. Nonsqaure $\mathbf{A}$ such as the one we just saw, require the pseudoinverse,

$$\mathbf{A}^{\dagger} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T. \tag{17}$$

Sometimes solving $\mathbf{Ax} + \mathbf{b} = 0$ is implossible, the pseudoinverse considers,

$$\min_x \frac{1}{2}|\mathbf{Ax} - \mathbf{b}|^2 \tag{18}$$

$$\tag{19}$$

instead. $\mathbf{A}^{\dagger}\mathbf{b} = \mathbf{x}$ yields the solution.

Sometimes solving $\mathbf{Ax} + \mathbf{b} = 0$ is implossible. One the board, derive:

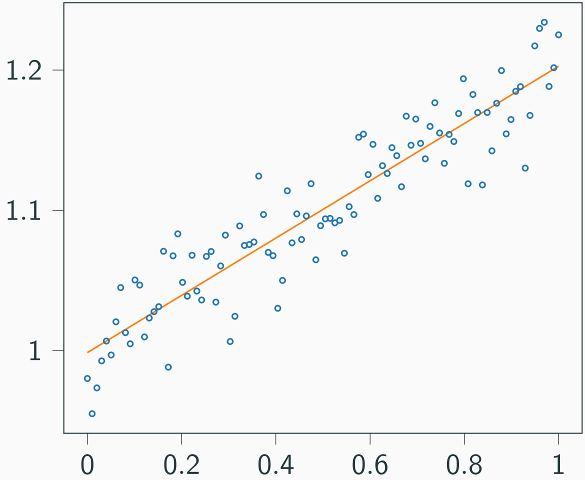
$$\min_x \frac{1}{2}|\mathbf{Ax} - \mathbf{b}|^2 \tag{20}$$

$$\tag{21}$$

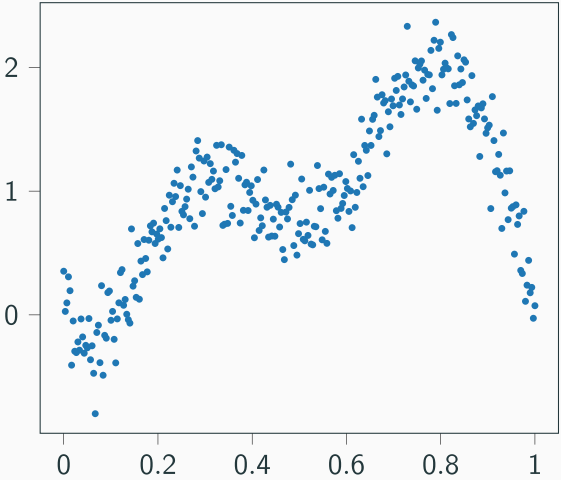
At the optimum we expect,

$$
\begin{aligned}
0 &= \nabla_x \frac{1}{2}|\mathbf{Ax} - \mathbf{b}|^2 && (22)\\
&= \nabla_x \frac{1}{2}(\mathbf{Ax} - \mathbf{b})^T(\mathbf{Ax} - \mathbf{b}) && (23)\\
&= (\mathbf{Ax} - \mathbf{b})\mathbf{A}^T && (24)\\
&= \mathbf{A}^T\mathbf{Ax} - \mathbf{A}^T\mathbf{b} && (25)\\
\mathbf{A}^T\mathbf{b} &= \mathbf{A}^T\mathbf{Ax} && (26)\\
(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{b} &= \mathbf{x} && (27)
\end{aligned}
$$

Linear regression



What about harder problems?



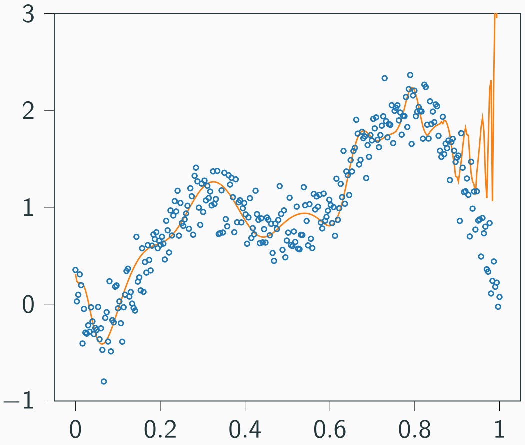
Fitting higher order polynomials

$$\underbrace{\begin{pmatrix} 1 & x_1^1 & x_1^2 & \dots & x_1^m \\ 1 & x_2^1 & x_2^2 & \dots & x_2^m \\ 1 & x_3^1 & x_3^2 & \dots & x_3^m \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n^1 & x_n^2 & \dots & x_n^m \end{pmatrix}}_{\mathbf{A}} \underbrace{\begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{pmatrix}}_{\mathbf{x}} = \underbrace{\begin{pmatrix} p_1 \\ p_2 \\ \vdots \\ p_n \end{pmatrix}}_{\mathbf{b}}. \tag{28}$$

As we saw for the linear regression $\mathbf{A}^\dagger \mathbf{b} = \mathbf{x}$ gives us the coefficients.

Overfitting

Below the solution for a polynomial of 7th degree, that is $m = 7$.



The noise took over! What now?

Regularization

Motivation

- Is there a way to fix the previous example?
- To do so we start from a rather peculiar observation.

Eigenvalues and Eigen-Vectors

Multiply matrix $\mathbf{A}$ with vectors $\mathbf{x_1}$ and $\mathbf{x_2}$,

$$\mathbf{A} = \begin{pmatrix} 1 & 4 \\ 0 & 2 \end{pmatrix}, \mathbf{x_1} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \mathbf{x_2} = \begin{pmatrix} 4 \\ 1 \end{pmatrix}, \tag{29}$$

we observe

$$\mathbf{Ax_1} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \mathbf{Ax_2} = \begin{pmatrix} 8 \\ 2 \end{pmatrix} \tag{30}$$

Vector $\mathbf{x_1}$ has not changed! Vector $\mathbf{x_2}$ was multiplied by two. In other words,

$$\mathbf{Ax_1} = 1\mathbf{x_1}, \mathbf{Ax_2} = 2\mathbf{x_2} \tag{31}$$

Eigenvalues and Eigenvectors

Eigenvectors turn multiplication with a matrix into multiplication with a number,

$$\mathbf{A}\mathbf{x} = \lambda \mathbf{x}. \tag{32}$$

Subtracting $\lambda \mathbf{x}$ leads to,

$$(\mathbf{A}\mathbf{x} - \lambda \mathbf{I})\mathbf{x} = 0 \tag{33}$$

$$\tag{34}$$

The interestin solutions are those were $\mathbf{x} \neq 0$, which means

$$\det(\mathbf{A} - \lambda \mathbf{I}) = 0 \tag{35}$$

Eigenvalues and Eigenvectors

Eigenvectors turn multiplication with a matrix into multiplication with a number,

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x}. \tag{32}$$

Subtracting $\lambda\mathbf{x}$ leads to,

$$(\mathbf{A}\mathbf{x} - \lambda\mathbf{I})\mathbf{x} = 0 \tag{33}$$

(34)

The interestin solutions are those were $\mathbf{x} \neq 0$, which means

$$\det(\mathbf{A} - \lambda\mathbf{I}) = 0 \tag{35}$$

On the board, compute the eigenvalues and vectors for the initial example.

TODO: write down.

Eigenvalue-Decomposition [Str+09]

Eigenvalues let us look into the heart of a sqaure system-matrix $\mathbf{A} \in \mathbb{R}^{n,n}$.

$$\mathbf{A} = \mathbf{S} \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{pmatrix} \mathbf{S}^{-1} = \mathbf{S}\Lambda\mathbf{S}^{-1}, \tag{36}$$

with $\mathbf{S} \in \mathbb{R}^{n,n}$ and $\Lambda \in \mathbb{C}^{n,n}$.

Singular-Value-Decomposition [Str+09]

What about a non-square matrix $\mathbf{A} \in \mathbb{R}^{n,m}$? Idea:

$$\mathbf{A^T A} = \mathbf{V} \begin{pmatrix} \sigma_1^2 & & \\ & \ddots & \\ & & \sigma_n^2 \end{pmatrix} \mathbf{V}^{-1}, \mathbf{AA^T} = \mathbf{U} \begin{pmatrix} \sigma_1^2 & & \\ & \ddots & \\ & & \sigma_n^2 \end{pmatrix} \mathbf{U}^{-1}. \tag{37}$$

Using the eigenvectors of the $\mathbf{A}^T\mathbf{A}$ and $\mathbf{A}\mathbf{A}^T$ we construct,

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T, \tag{38}$$

with $\mathbf{A} \in \mathbb{R}^{m,n}$, $\mathbf{U} \in \mathbb{R}^{m,m}$, $\boldsymbol{\Sigma} \in \mathbb{R}^{m,n}$ and $\mathbf{V} \in \mathbb{R}^{n,n}$.

Singular values and matrix inversion [GK65]

$$\mathbf{A}^{\dagger} = \mathbf{V}\Sigma^{\dagger}\mathbf{U}^{T} = \mathbf{V}\left(\begin{array}{ccc} \sigma_1^{-1} & & \\ & \ddots & \\ & & \sigma_m^{-1} \\ \hline & 0 & \end{array}\right)\mathbf{U}^{T} \tag{39}$$

Regularization via Singular Value Filtering

Originally we had a problem computing $\mathbf{A}^{\dagger}\mathbf{b} = \mathbf{x}$. To solve it, we compute,

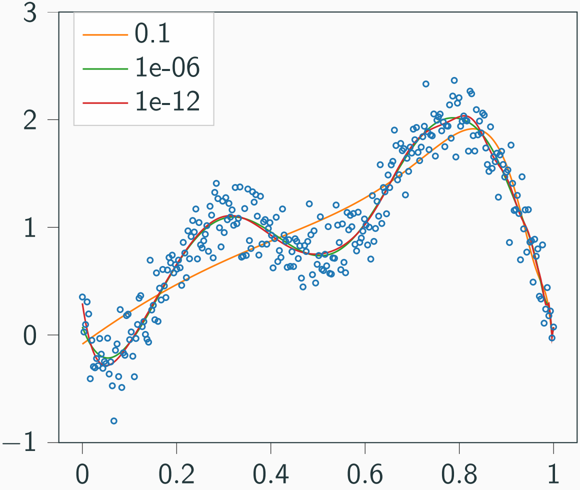
$$\mathbf{x}_{reg} = \sum_{i=1}^{n} f_i \frac{\mathbf{u}_i^T b}{\sigma_i} \mathbf{v_i} \tag{40}$$

The filter factors are computed using $f_i = \sigma_i^2/(\sigma_i^2 + \epsilon)$. Singular values $\sigma_i < \epsilon$ are filtered. Expressing equation 40 using matrix notation:

$$\mathbf{x}_{reg} = \mathbf{VF} \left(\begin{array}{ccc} \sigma_1^{-1} & & \\ & \ddots & \\ & & \sigma_m^{-1} \\ \hline & 0 & \end{array} \right) \mathbf{U}^T \mathbf{b}_{noise} \tag{41}$$

with $\mathbf{A} \in \mathbb{R}^{m,n}$, $\mathbf{U} \in \mathbb{R}^{m,m}$, $\mathbf{V} \in \mathbb{R}^{n,n}$, $\mathbf{F} \in \mathbb{R}^{m,m}$, $\Sigma^{\dagger} \in \mathbb{R}^{n,m}$ and $\mathbf{b} \in \mathbb{R}^{n,1}$.

Regularized solution



Conclusion

- True scientists know what linear can do for them!
- Think about matrix shapes. If you are solving a problem, rule out all formulations where the shapes don't work.
- Regularization using the SVD is also known as Tikhonov regularization.

References

[DFO20] Marc Peter Deisenroth, A Aldo Faisal, and Cheng Soon Ong. *Mathematics for machine learning*. Cambridge University Press, 2020.

[GK65] Gene Golub and William Kahan. "Calculating the singular values and pseudo-inverse of a matrix." In: *Journal of the Society for Industrial and Applied Mathematics, Series B: Numerical Analysis* 2.2 (1965), pp. 205–224.

[Str+09] Gilbert Strang, Gilbert Strang, Gilbert Strang, and Gilbert Strang. *Introduction to linear algebra*. Vol. 4. Wellesley-Cambridge Press Wellesley, MA, 2009.