Linear Algebra for Machine Learning

Moritz Wolter

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High-Performance Computing and Analytics Lab, University of Bonn

Overview

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

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

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

Multiplication

Multiplying $\mathbf{A} \in \mathbb{R}^{m,n}$ 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,

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

The identity matrix

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

Matrix inverse

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

$$\mathbf{A}\mathbf{A}^{-1} = \mathbf{I}. \tag{6}$$

The process of computing the inverse is called Gaussian elimination.

The Transpose

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

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^T = \begin{pmatrix} a & c \\ b & d \end{pmatrix} \tag{7}$$

Motivation of the determinant

- The determinant contains lots of information about a matrix in a single number.
- When a matrix has a zero determinant, a column is a linear combination of other columns. Its inverse does not exist.
- We require determinants to find eigenvalues by hand.

Computing determinants in two or three dimensions

The two-dimensional case:

$$\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11} \cdot a_{22} - a_{12} \cdot a_{21} \tag{8}$$

$$\tag{9}$$

Computing the determinant of a three-dimensional matrix.

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = a_{11} \cdot \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} - a_{21} \cdot \begin{vmatrix} a_{12} & a_{13} \\ a_{32} & a_{33} \end{vmatrix} + a_{31} \cdot \begin{vmatrix} a_{12} & a_{13} \\ a_{22} & a_{23} \end{vmatrix} \tag{10}$$

Determinants in n-dimensions

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

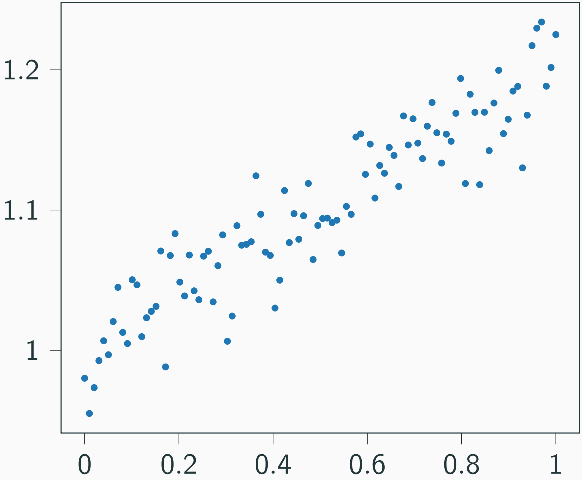
$$\dots a_{m1} \begin{vmatrix} a_{11} & \dots & a_{1n} \\ a_{21} & \dots & a_{2n} \\ \vdots & & \vdots \end{vmatrix}$$

Summary

- We saw some of the most important operations in linear algebra.
- Let's use these to do something useful next.

Linear curve fitting

What is the best line connecting measurements?



Problem Formulation

A line has the form $f(a) = da + c$, with $c, a, d \in \mathbb{R}$. In matrix language, we could ask for every point to be on the line,

$$\begin{pmatrix} 1 & a_1 \\ 1 & a_2 \\ 1 & a_3 \\ \vdots & \vdots \\ 1 & a_n \end{pmatrix} \begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} p_1 \\ p_2 \\ \vdots \\ p_n \end{pmatrix}. \tag{11}$$

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 exists for square or n by n matrices. Nonsquare $\mathbf{A}$ such as the one we just saw, require the pseudoinverse,

$$\mathbf{A}^{\dagger} = (\mathbf{A}^{T}\mathbf{A})^{-1}\mathbf{A}^{T}. \tag{12}$$

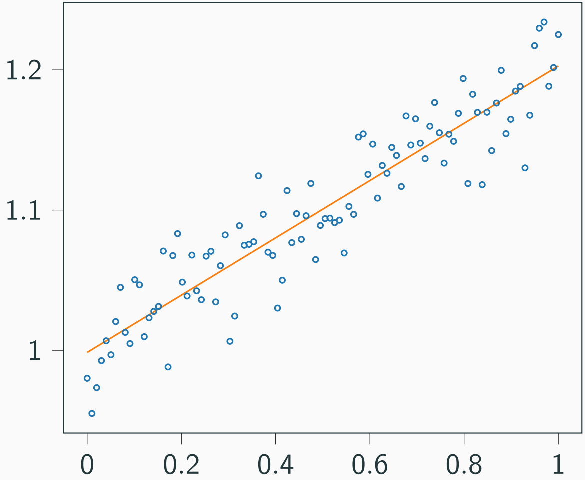
Sometimes solving $\mathbf{A}\mathbf{x} - \mathbf{b} = 0$ is impossible, the pseudoinverse considers,

$$\min_{x} \frac{1}{2}|\mathbf{A}\mathbf{x} - \mathbf{b}|^{2} \tag{13}$$

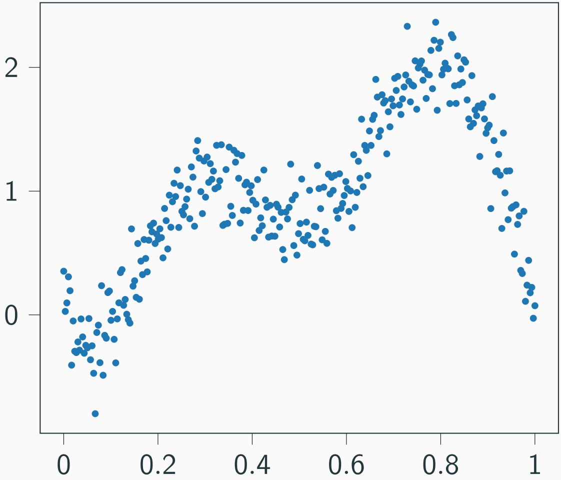
$$\tag{14}$$

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

Linear regression



What about harder problems?



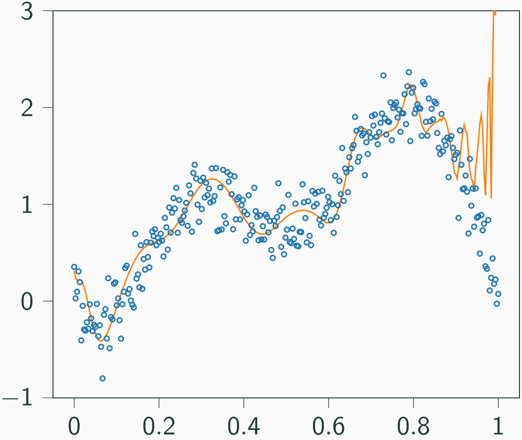
Fitting higher order polynomials

$$\underbrace{\begin{pmatrix} 1 & a_1^1 & a_1^2 & \dots & a_1^m \\ 1 & a_2^1 & a_2^2 & \dots & a_2^m \\ 1 & a_3^1 & a_3^2 & \dots & a_3^m \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & a_n^1 & a_n^2 & \dots & a_n^m \end{pmatrix}}_{\mathbf{A}} \underbrace{\begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{pmatrix}}_{\mathbf{x}} = \underbrace{\begin{pmatrix} p_1 \\ p_2 \\ \vdots \\ p_n \end{pmatrix}}_{\mathbf{b}}. \tag{15}$$

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

Overfitting

The figure below depicts the solution for a polynomial of 7th degree, that is $m = 7$.



Summary

- We saw how linear algebra lets us fit polynomials to curves.
- For the 7th-degree polynomial the noise took over! What now?

Regularization

Motivation

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

Eigenvalues and Eigen-Vectors

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

$$\mathbf{A} = \begin{pmatrix} 1 & 4 \\ 0 & 2 \end{pmatrix}, \mathbf{x_1} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \mathbf{x_2} = \begin{pmatrix} 4 \\ 1 \end{pmatrix}, \tag{16}$$

we observe

$$\mathbf{Ax_1} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \mathbf{Ax_2} = \begin{pmatrix} 8 \\ 2 \end{pmatrix} \tag{17}$$

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

$$\mathbf{Ax_1} = 1\mathbf{x_1}, \mathbf{Ax_2} = 2\mathbf{x_2} \tag{18}$$

Eigenvalues and Eigenvectors

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

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x}. \tag{19}$$

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

$$(\mathbf{A} - \lambda\mathbf{I})\mathbf{x} = 0 \tag{20}$$

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

$$\det(\mathbf{A} - \lambda\mathbf{I}) = 0 \tag{21}$$

Eigenvalue-Decomposition [Str+09]

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

$$\mathbf{A} = \mathbf{S} \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{pmatrix} \mathbf{S}^{-1} = \mathbf{S}\Lambda\mathbf{S}^{-1}, \qquad (22)$$

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

Singular-Value-Decomposition [Str+09]

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

$$\mathbf{A^T A} = \mathbf{V} \begin{pmatrix} \sigma_1^2 & & \\ & \ddots & \\ & & \sigma_n^2 \end{pmatrix} \mathbf{V}^{-1}, \mathbf{A A^T} = \mathbf{U} \begin{pmatrix} \sigma_1^2 & & \\ & \ddots & \\ & & \sigma_m^2 \end{pmatrix} \mathbf{U}^{-1}. \tag{23}$$

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

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T, \tag{24}$$

with $\mathbf{A} \in \mathbb{R}^{m,n}$, $\mathbf{U} \in \mathbb{R}^{m,m}$, $\Sigma \in \mathbb{R}^{m,n}$ and $\mathbf{V} \in \mathbb{R}^{n,n}$. Σ's diagonal is filled with the square root $\mathbf{A}^T\mathbf{A}$'s eigenvalues.

Singular values and matrix inversion [GK65]

The singular value matrix is a zero-padded diagonal matrix

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T = \mathbf{U}\begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \\ \hline & 0 & \end{pmatrix}\mathbf{V}^T. \tag{25}$$

Inverting the sigmas and transposing yields the pseudoinverse

$$\mathbf{A}^\dagger = \mathbf{V}\Sigma^\dagger\mathbf{U}^T = \mathbf{V}\begin{pmatrix} \sigma_1^{-1} & & \\ & \ddots & \\ & & \sigma_n^{-1} \\ \hline & 0 & \end{pmatrix}^T \mathbf{U}^T. \tag{26}$$

Regularization via Singular Value Filtering

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

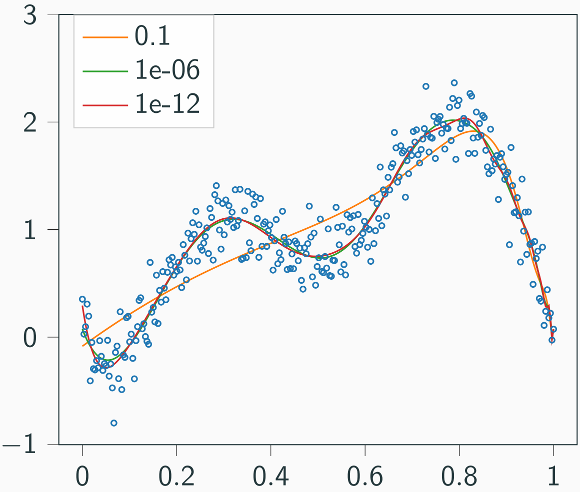
$$\mathbf{x}_{reg} = \sum_{i=1}^{n} f_i \frac{\mathbf{u}_i^T b}{\sigma_i} \mathbf{v_i} \tag{27}$$

The filter factors are computed using $f_i = \sigma_i^2/(\sigma_i^2 + \epsilon)$. Singular values $\sigma_i < \epsilon$ are filtered. Expressing equation 27 using matrix notation:

$$\mathbf{x}_{reg} = \mathbf{V}\mathbf{F}\Sigma^\dagger \mathbf{U}^T \mathbf{b}_{noise} \tag{28}$$

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

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.