

Let's take a look at the simple 2d data. We have a set of blue points on the plane. We can easily see that the projections on the first axis (red dots) have maximum variance at the final position of the animation. The second (and the last) axis should be orthogonal to the previous one.



This idea could be used in a variety of ways. For example, it might happen, that projection of complex data on the principal plane (only 2 components) bring you enough intuition for clustering. The picture below plots projection of the labeled dataset onto the first to principal components (PCs), we can clearly see, that only two vectors (these PCs) would be enogh to differ Finnish people from Italian in particular dataset (celiac disease (Dubois et al. 2010)) source

eeu 370 netak

buag

a: er

Problem

The first component should be defined in order to maximize variance. Suppose, we've already normalized the data, i.e. $\sum_{i} a_i = 0$, then sample variance will become the sum



$$egin{aligned} A^ op A &= (W\Sigma U^ op)(U\Sigma V^ op) \ &= W\Sigma I\Sigma W^ op \ &= W\Sigma \Sigma W^ op \ &= W\Sigma \Sigma W^ op \ &= W\Sigma^2 W^ op \end{aligned}$$

Which corresponds to the eigendecomposition of matrix $A^{\top}A$, where W stands for the matrix of eigenvectors of $A^{\top}A$, while Σ^2 contains eigenvalues of $A^{\top}A$. $A = U Z W^{T}$

UZW

At the end:

The latter formula provide us with easy way to compute PCA via SVD with any number npockyuu nep bul of principal components:

$$\begin{split} & \Pi = A \cdot W = \\ & \underset{\scriptstyle \mathsf{mx}}{\overset{\scriptstyle \mathsf{mx}}}{\overset{\scriptstyle \mathsf{mx}}}{\overset{\scriptstyle \mathsf{mx}}}{\overset{\scriptstyle \mathsf{mx}}{\overset{\scriptstyle \mathsf{mx}}}{\overset{\scriptstyle \mathsf{mx}}}}}}}}}}}}}}}}}}}}}} } \\{ = U \Sigma W {}^{\mathsf{mx}} {}^{\mathsf{mx}} {}^{\mathsf{mx}} {}^{\mathsf{mx}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}} {}^{\mathsf{mx}} {}^{\mathsf{mx}} {}^{\mathsf{mx}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}} {}^{\mathsf{mx}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}}} {}^{\mathsf{mx}} {}^{\mathsf{mx}} {}$$

$$\Pi_r = U_r \Sigma_r$$
 PC

Examples

送 Iris dataset

Consider the classical Iris dataset



(2) npoeky..... $\Pi_r = U_r \cdot Z_r$



source We have the dataset matrix $A \in \mathbb{R}^{150 imes 4}$





Code

CO Open in Colab

Related materials

- Wikipedia
- Blog post
- Blog post

Useful definitions and notations

We will treat all vectors as column vectors by default. The space of real vectors of length n is denoted by \mathbb{R}^n , while the space of real-valued $m \times n$ matrices is denoted by $\mathbb{R}^{m \times n}$.

Basic linear algebra background

The standard **inner product** between vectors x and y from \mathbb{R}^n is given by

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

Here x_i and y_i are the scalar *i*-th components of corresponding vectors.

The standard **inner product** between matrices X and Y from $\mathbb{R}^{m imes n}$ is given by

$$\langle X,Y
angle = \mathrm{tr}(X^ op Y) = \sum_{i=1}^m \sum_{j=1}^n X_{ij}Y_{ij} = \mathrm{tr}(Y^ op X) = \langle Y,X
angle$$

The determinant and trace can be expressed in terms of the eigenvalues

$${
m det} A = \prod_{i=1}^n \lambda_i, \qquad {
m tr} A = \sum_{i=1}^n \lambda_i$$

Don't forget about the cyclic property of a trace for a square matrices A, B, C, D:

$$\operatorname{tr}(ABCD) = \operatorname{tr}(DABC) = \operatorname{tr}(CDAB) = \operatorname{tr}(BCDA)$$

The largest and smallest eigenvalues satisfy

$$\lambda_{\min}(A) = \inf_{x
eq 0} rac{x^ op A x}{x^ op x}, \qquad \lambda_{\max}(A) = \sup_{x
eq 0} rac{x^ op A x}{x^ op x}$$

and consequently $orall x \in \mathbb{R}^n$ (Rayleigh quotient):

$$\lambda_{\min}(A)x^ op x \leq x^ op Ax \leq \lambda_{\max}(A)x^ op x$$

A matrix $A \in \mathbb{S}^n$ (set of square symmetric matrices of dimension n) is called **positive** (semi)definite if for all $x \neq 0$ (for all x) : $x^{\top}Ax > (\geq)0$. We denote this as



Let A be a matrix of size $m \times n$, and B be a matrix of size $n \times p$, and let the product AB be:

$$C = AB$$

then C is a $m \times p$ matrix, with element (i, j) given by:

$$c_{ij} = \sum_{k=1}^n a_{ik} b_{kj}$$

Let A be a matrix of shape $m \times n$, and x be $n \times 1$ vector, then the i-th component of the product:

$$z = Ax$$

is given by:

$$z_i = \sum_{k=1}^n a_{ik} x_k$$

Finally, just to remind:

- C = AB $C^{\top} = B^{\top}A^{\top}$
- $AB \neq BA$
- $e^A = \sum_{k=0}^\infty rac{1}{k!} A^k$
- $e^{A+B} \neq e^A e^B$ (but if A and B are commuting matrices, which means that $AB = BA, e^{A+B} = e^A e^B$)
- $\langle x,Ay
 angle = \langle A^ op x,y
 angle$

Gradient

Let $f(x) : \mathbb{R}^n \to \mathbb{R}$, then vector, which contains all first order partial derivatives:

$$abla f(x) = rac{df}{dx} = egin{pmatrix} rac{\partial f}{\partial x_1} \ rac{\partial f}{\partial x_2} \ dots \ rac{\partial f}{\partial x_n} \end{pmatrix}$$

named gradient of f(x). This vector indicates the direction of steepest ascent. Thus, vector $-\nabla f(x)$ means the direction of the steepest descent of the function in the point. Moreover, the gradient vector is always orthogonal to the contour line in the point.

Hessian

Let $f(x): \mathbb{R}^n \to \mathbb{R}$, then matrix, containing all the second order partial derivatives:

$$f''(x) = \frac{\partial^2 f}{\partial x_i \partial x_j} = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_n} \end{pmatrix}$$

In fact, Hessian could be a tensor in such a way: $(f(x) : \mathbb{R}^n \to \mathbb{R}^m)$ is just 3d tensor, every slice is just hessian of corresponding scalar function $(H(f_1(x)), H(f_2(x)), \dots, H(f_m(x))).$

Jacobian

The extension of the gradient of multidimensional $f(x): \mathbb{R}^n \to \mathbb{R}^m$ is the following matrix:

$$f'(x) = rac{df}{dx^T} = egin{pmatrix} rac{\partial f_1}{\partial x_1} & rac{\partial f_1}{\partial x_2} & \cdots & rac{\partial f_1}{\partial x_n} \ rac{\partial f_2}{\partial x_1} & rac{\partial f_2}{\partial x_2} & \cdots & rac{\partial f_2}{\partial x_n} \ dots & dots & \ddots & dots \ rac{\partial f_m}{\partial x_1} & rac{\partial f_m}{\partial x_2} & \cdots & rac{\partial f_m}{\partial x_n} \end{pmatrix}$$

Summary

	f(x):X ightarrow Y;	$\frac{\partial f(x)}{\partial x}\in G$	
х	Υ	G	Name
\mathbb{R}	\mathbb{R}	\mathbb{R}	$f^{\prime}(x)$ (derivative)
\mathbb{R}^{n}	\mathbb{R}	\mathbb{R}^n	$rac{\partial f}{\partial x_i}$ (gradient)
\mathbb{R}^{n}	\mathbb{R}^m	$\mathbb{R}^{m imes n}$	$rac{\partial f_i}{\partial x_j}$ (jacobian)
$\mathbb{R}^{m imes n}$	\mathbb{R}	$\mathbb{R}^{m imes n}$	$rac{\partial f}{\partial x_{ij}}$

General concept

Naive approach

The basic idea of naive approach is to reduce matrix/vector derivatives to the wellknown scalar derivatives.

Matrix notation of a function

$$f(x) = c^{\top} x$$

Scalar notation of a function

$$f(x) = \sum_{i=1}^{n} c_i x_i$$

Matrix notation of a gradient

$$\nabla f(x) = c$$

$$\uparrow$$

$$\frac{\partial f(x)}{\partial x_k} = c_k$$

Simple derivative

$$\frac{\partial f(x)}{\partial x_k} = \frac{\partial \left(\sum_{i=1}^n c_i x_i\right)}{\partial x_k}$$

One of the most important practical tricks here is to separate indices of sum (i) and

partial derivatives (k). Ignoring this simple rule tends to produce mistakes.

Differential approach

The guru approach implies formulating a set of simple rules, which allows you to calculate derivatives just like in a scalar case. It might be convenient to use the $f: \mathbb{R}^n \rightarrow \mathbb{R}$ differential notation here.

df = f(x+dx) - f(x)

Differentials

sagara: After obtaining the differential notation of df we can retrieve the gradient using normal following formula: $df(x) = \langle
abla f(x), dx
angle$ Nociut AT6

||dx||→0

2) Nov

Then, if we have differential of the above form and we need to calculate the second derivative of the matrix/vector function, we treat "old"
$$dx$$
 as the constant dx_1 , then calculate $d(df) = d^2 f(x)$

$$d^2f(x) = \langle \nabla^2 f(x) dx_1, dx \rangle = \langle H_f(x) dx_1, dx \rangle$$
 df = $\langle \dots, dx \rangle$
3)

Properties

Let A and B be the constant matrices, while X and Y are the variables (or matrix functions).

$$dA = 0$$

 $d(\alpha X) = \alpha(dX)$
 $d(AXB) = A(dX)B$
 $d(X+Y) = dX + dY$
 $d(X^{\top}) = (dX)^{\top}$
 $d(XY) = (dX)Y + X(dY)$
 $d\langle X, Y \rangle = \langle dX, Y \rangle + \langle X, dY \rangle$
 $d\left(\frac{X}{\phi}\right) = \frac{\phi dX - (d\phi)X}{\phi^2}$
 $d(\det X) = \det X \langle X^{-\top}, dX \rangle$
 $d(\operatorname{tr} X) = \langle I, dX \rangle$
 $df(g(x)) = \frac{df}{dg} \cdot dg(x)$
 $H = (J(\nabla f))^T$

$\begin{array}{c} \boxed{Perretue} 1 & f(x) = X ^2 & \nabla f = ? \\ \hline{f: R' \to R} \end{array}$	≠fe R'
1) $df = d(X ^2) = d(\langle X, X \rangle) =$	
$= \langle dx, x \rangle + \langle x, dx \rangle = \langle x, dx \rangle + \langle x, dx \rangle$	
$\rightarrow \nabla f = 2 \times e R^{h}$	
Ynp. 1 $f(x) = X _F^2$, $X \in \mathbb{R}^{m \times n} \nabla$ Permetrice: ∇	f = ? $f \in \mathbb{R}^{m \times n}$
$df = d(X _{F}^{2}) = d(\langle X, X \rangle) =$	•
$= \langle dX, X \rangle + \langle X, dX \rangle = 2 \langle X, dX \rangle$	X > =
$= \langle 2 \times 0 \times 7 = > \vee 7$	Rafin
$\begin{array}{rcl} \hline & \Pi pumep \ 2 \end{array} & f(x) = \frac{1}{2} x^{T} A x - b^{T} x + C & f: \mathbb{R}^{2} - \mathcal{T} f = $	→ R P ^{**} be P
Pennenne: s) $df = d(\frac{1}{2}xAx - bx+c) = X$	Y = (x, y)
$= d(\frac{1}{2} \langle x, Ax \rangle - \langle D, x \rangle + C) =$ = $d(\frac{1}{2} \langle x, Ax \rangle) - d(\langle b, x \rangle) + d(C) =$	

 $= \frac{1}{2}((dx,Ax) + (x,ol(Ax))) - (db,x) - (dx,b) + 0 =$ B HYXHOU DOPME = $\frac{1}{2}((Ax, olx) + (x, Adx)) - (b, olx) =$ nopasona $= \frac{1}{2} \left(\langle A \times, d \times \rangle + \langle A \times, d \times \rangle \right) - \langle b, d \times \rangle =$ $=\frac{1}{2}\langle Ax+Ax, dx\rangle - \langle b, dx\rangle =$ $= \langle \pm (A+A^{T})_{x} - b_{y} dx \rangle$ $\nabla f => \nabla f = \frac{1}{2}(A + A)x b$ eem $A \geq 0 => A = A^T$ $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}' \rightarrow \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ $\nabla f = Ax - b$ Ynp 2 3agara Nux. perpeceu e lz perynapuzau $f(x) = ||Ax-b||^2 + \frac{1}{2}||X||^2 \quad f: \mathbb{R}^n \to \mathbb{R}$ $\nabla f=?$ Penerue 1) $df = d(||Ax-b||^2 + \frac{\lambda}{2}||x||^2) =$ $= d(IAx - bII) + d(\frac{\lambda}{2}IIXII) =$ $\leq \frac{1}{2} d(IXI) =$ $= d(\langle y, y \rangle) = Ax - b$ = 2 \langle y, dy \rangle = dy = d(Ax - b) = dy = d(Ax - b) = dx = Adx $=\frac{\lambda}{2}d(x,x)=$ $= \frac{\lambda}{2} \cdot 2\langle X, dX \rangle =$ $= \langle \lambda X, dX \rangle$

= $\langle 2(Ax-b), Adx \rangle =$ = < 2AT(Ax-b), dx> $\nabla f = \lambda x + 2A(Ax-b) \in \mathbb{R}^{n}$ $\nabla f = ? \in \mathbb{R}^{n \times n}$ $Y_{np.} \quad f(x) = tr(X)$ $\langle X, Y \rangle = tr(X^T Y)$ i) df = d(tr(X)) == $tr(Y^{T}X)$ = d(tr(IX)) = $= d\left(\langle X, \underline{I}^{\dagger} \rangle\right) = \langle dX, I \rangle + \langle X, dI \rangle =$ =<I,dX> => \[\nabla f = I \] Mos negrance our to F. KAK CRUTATE F'=? $df = \langle \nabla f, dx \rangle$ KAK CUUTATE f"? V°f s) $df = \langle \nabla f, dx \rangle$ $dx := dx_1$ crutaeu $dx_1 = const$ 2) $d(df) = d^2 f = d(\langle \nabla f, dx_1 \rangle) =$ $= \langle d(\nabla f), dx_1 \rangle = f''$ 3) Noubern & Bugy: d2f=<(...dx,dx)

 $f(x) = \frac{1}{2}x^{T}Ax - b^{T}x + C$ Nouvep: $df = \langle \frac{1}{2}(A+A)x - b, dx \rangle$; **t**) $dx = dx_1$ 2) Crucaese $d^2f = d(\langle \frac{1}{2}(A+A)x - b, dx_y \rangle) =$ = $\left(d\left(\frac{1}{2}(A+A^{T})x-b\right),dx_{s}\right)$ db=0 $= \langle \pm d((A+A^{T})x), dx_{1} \rangle =$ = $\langle \frac{1}{2} (A + A) | dx, dx_1 \rangle = f'' = \frac{1}{2} (A + A')$ MATE dx, dx_3 T, T $(A + A^{T}) = A^{T} + A =$ $= A + A^{T}$ $= \langle dx, \frac{1}{2}(A+A^{T})dx_{1}\rangle_{=}$ $= \langle \frac{1}{2} (A + A) dx_1, dx \rangle$ f"= ? $f(x) = ||Ax-b||^2 + \frac{1}{2}||X|^2$ Ynp. MEHSey $df = (2A'(Ax-b) + \lambda x, dx)$ Pemetue: dx "dx $d^2 f = \langle \dots dx, dx \rangle$ $f) d(df) = d^2f =$ ATOM. = $\langle d(2A^{T}(Ax-b)+\lambda x), dx_{1} \rangle =$ (=)

 $a(\lambda \times) = \lambda \cdot dx$ $2\overline{A} \cdot d(A \times -b) =$ $= 2 A^{T} \cdot (d(A_{x}) - 0) =$ = 2AT · Adx $(A^{T}A)' =$ = < 2ATA dx + hdx, dx1>= = $\langle (2A^TA + \lambda I) dx, dx_1 \rangle$ $= A^T A^T =$ I.V=V $= \mathbf{A}^{\mathsf{T}} \mathbf{A}$ Y dx = y. I. dx $\int_{a}^{n} = 2\bar{A}A + \lambda I$ $\|c\| \times \| \to 0$ d(dx) = 1e - 5 $(dx)^{2} = 1e - 10$ d(f(x), dx) = $= \langle df^{}, dx > + \langle f^{}, d(dx) >$

 $d(X^{-1}) = -X^{-1}(dX)X^{-1}$

References

- Convex Optimization book by S. Boyd and L. Vandenberghe Appendix A.
 Mathematical background.
- Numerical Optimization by J. Nocedal and S. J. Wright. Background Material.
- Matrix decompositions Cheat Sheet.
- Good introduction
- The Matrix Cookbook
- MSU seminars (Rus.)
- Online tool for analytic expression of a derivative.
- Determinant derivative