#### Problem Linear least squares Linear least squares  $10$  $10$ Function value Function value  $\overline{5}$  $\overline{5}$  $\overline{0}$  $-10.0$   $-7.5$   $-5.0$   $-2.5$  0.0 2.5  $-7.5$   $-5.0$   $-2.5$  0.0 2.5  $5.0$ 7.5

In a least-squares, or linear regression, problem, we have measurements  $X \in \mathbb{R}^{m \times n}$ and  $y\in\mathbb{R}^m$  and seek a vector  $\theta\in\mathbb{R}^n$  such that  $\bm{X}\theta$  is close to  $y.$  Closeness is defined Had Mogencer as the sum of the squared differences:



For example, we might have a dataset of  $m$  users, each represented by  $n$  features Each row  $x_i^{\top}$  of  $X$  is the features for user  $i$ , while the corresponding entry  $y_i$  of  $y$  is the measurement we want to predict from  $x_i^\top$ , such as ad spending. The prediction is given  $\mu$ BOINYKRAA  $f(x) = x$ by  $x_i^{\top}\theta$ .

We find the optimal  $\theta$  by solving the optimization problem

 $||X\theta - y||_2^2 \rightarrow \min_{\theta \in \mathbb{R}^n}$ 

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Let  $\theta^*$  denote the optimal  $\theta$ . The quantity  $r = X\theta^* - y$  is known as the residual. If  $||r||_2 = 0$ , we have a perfect fit.  $||\mathbf{X}|| = |\mathbf{X}||_2 =$ **DEWICH US**  $\|x\|_4$ ,  $\|x\|_{\infty}$ ,  $\|x\|_{\infty}$ p31 Note, that the function needn't be linear in the argument  $x$  but only in the para

Xθ

that are to be determined in the best fit.



## Approaches

### Moore–Penrose inverse

If the matrix  $X$  is relatively small, we can write down and calculate exact solution:

$$
\theta^* = (X^\top X)^{-1} X^\top y = X^\dagger y,
$$

where  $X^\dagger$  is called pseudo-inverse matrix. However, this approach squares the condition number of the problem, which could be an obstacle in case of ill-conditioned huge scale problem.

## QR decomposition

For any matrix  $X \in \mathbb{R}^{m \times n}$  there is exists QR decomposition:

$$
X=Q\cdot R,
$$

where  $Q$  is an orthogonal matrix (its columns are orthogonal unit vectors meaning  $Q^\top Q = QQ^\top = I$  and  $R$  is an upper triangular matrix. It is important to notice, that since  $Q^{-1} = Q^\top$  , we have:

 $QR\theta = y \rightarrow R\theta = Q^{\top}y$ 

Now, process of finding theta consists of two steps:

- 1 Find the QR decomposition of *X*.
- $2$   $\,$  Solve triangular system  $R\theta = Q^\top y$ , which is triangular and, therefore, easy to solve.

## Cholesky decomposition

For any positive definite matrix  $A \in \mathbb{R}^{n \times n}$  there is exists Cholesky decomposition:

$$
X^{\top} X = A = L^{\top} \cdot L,
$$

where  $L$  is an lower triangular matrix. We have:  $\,$ 

$$
L^\top L \theta = y \quad \longrightarrow \quad L^\top z_\theta = y
$$

Now, process of finding theta consists of two steps:

- 1 Find the Cholesky decomposition of  $X^{\top} X$ .
- 2 Find the  $z_{\theta} = L\theta$  by solving triangular system  $L^{\top}z_{\theta} = y$
- 3 Find the  $\theta$  by solving triangular system  $L\theta = z_{\theta}$

Note, that in this case the error stil proportional to the squared condition number.



#### Random square linear system



## **References**

- **CVXPY** documentation  $\bar{\theta}$
- Interactive example  $\sim$
- Jupyter notebook by A. Katrutsa  $\bar{\sigma}$

#### Applications / Minimum volume ellipsoid



Let  $x_1,\ldots,x_n$  be the points in  $\mathbb{R}^2.$  Given these points we need to find an ellipsoid, that contains all points with the minimum volume (in 2d case volume of an ellipsoin is just the square).

An invertible linear transformation applied to a unit sphere produces an ellipsoid with the square, that is  $\det A^{-1}$  times bigger, than the unit sphere square, that's why we parametrize the interior of ellipsoid in the following way:

$$
S=\{x\in\mathbb{R}^2\mid u=Ax+b, \|u\|_2^2\leq 1\}
$$

Sadly, the determinant is the function, which is relatively hard to minimize explicitly. However, the function  $\log \det A^{-1} = - \log \det A$  is actually convex, which provides a great opportunity to work with it. As soon as we need to cover all the points with ellipsoid of minimum volume, we pose an optimization problem on the convex function with convex restrictions:  $\overline{\Lambda}^2$  -  $\overline{\Lambda}$ 

$$
\min_{A \in \mathbb{R}^{2 \times 2}, b \in \mathbb{R}^2} - \log \det(A)
$$
\n  
\n
$$
\text{s.t. } ||Ax_i + b|| \le 1, i = 1, \dots, n \quad f(A) = \text{det }A
$$
\n
$$
A \succ 0
$$
\n
$$
f(A) = -\text{Lndet }A
$$





# **References**

- Jupyter notebook by A. Katrutsa
- https://cvxopt.org/examples/book/ellipsoids.html  $\bar{\phantom{a}}$

# Lipschitz constant of a convolutional layer in neural network

It was observed, that small perturbation in Neural Network input could lead to significant errors, i.e. misclassifications.



unu In this notebook we will try to estimate Lipschitz constant of some convolutional layer  $N$ uH. enoù Heù pohhoù<br>  $X_{in}$ <br>  $S(A = Y = W \cdot X_{in}$ <br>  $\|S(x+\epsilon) - S(x)\| \le L \|x+\epsilon - x\|$ <br>  $\|W(x+\epsilon) - Wx\| \le L \|E\|$ of a Neural Network.





Suppose, we have a set of  $n$  objects, which are needed to be splitted into two groups. Moreover, we have information about the preferences of all possible pairs of objects to be in the same group. this information could be presented in the matrix form:  $W \in \mathbb{R}^{n \times n}$ , where  $\{w_{ij}\}$  is the cost of having  $i$ -th and  $j$ -th object in the same partitions. It is easy to see, that the total number of partitions is finite and eqauls to  $2^n.$ So this problem can in principle be solved by simply checking the objective value of each feasible point. Since the number of feasible points grows exponentially, however, this is possible only for small problems (say, with  $n \leq 30$ ). In general (and for n larger than, say,  $50$ ) the problem is very difficult to solve.

For example, bruteforce solution on MacBook Air with M1 processor without any explicit parallelization will take more, than a universe lifetime for  $n=62.$ 



Despite the hardness of the problems, there are several ways to approach it.

# Problem

We consider the (nonconvex) problem min *<sup>x</sup>*∈R*<sup>n</sup> <sup>x</sup>*<sup>⊤</sup>*Wx*, s.t. *x*<sup>2</sup> *<sup>i</sup>* = 1, *i* = 1,…, *n* l

where  $W \in \mathbb{R}^n$  is the symetric matrix. The constraints restrict the values of  $x_i$  to  $1$  or  $-1$ , so the problem is equivalent to finding the vector with components  $\pm 1$  that  $m$ inimizes  $x^\top W x.$  The feasible set here is finite (it contains  $2^n$  points), thus, is nonconvex.

The objective is the total cost, over all pairs of elements, and the problem is to find the partition with least total cost.

## Simple lower bound with duality

We now derive the dual function for this problem. The Lagrangian is

$$
L(x,\nu)=x^\top W x+\sum_{i=1}^n\nu_i(x_i^2-1)=x^\top (W+\text{diag}(\nu))x-\mathbf{1}^\top\nu.
$$

We obtain the Lagrange dual function by minimizing over  $x$ :

$$
\begin{aligned} g(\nu) &= \inf_{x \in \mathbb{R}^n} x^\top (W + diag(\nu)) x - \mathbf{1}^\top \nu = \\ &= \begin{cases} \mathbf{1}^\top \nu, & W + \text{diag}(\nu) \succeq 0 \\ -\infty, & \text{otherwise} \end{cases} \end{aligned}
$$

sa

This dual function provides lower bounds on the optimal value of the difficult problem. For example, we can take any specific value of the dual variable

$$
\nu=-\lambda_{min}(W){\bf 1},
$$

This yields the bound on the optimal value  $p^\ast\colon$ 

$$
p^* \geq g(\nu) \geq -\mathbf{1}^\top\nu = n\lambda_{min}(W)
$$

Question Can you obtain the same lower bound without knowledge of duality, but using the iddea of eigenvalues?



## **References**

Convex Optimization book by Stephen Boyd and Lieven Vandenberghe. •

 $\sum_{i=1}^{n} (K X_i - Y_i)$  $L(k)$  $\frac{\partial L}{\partial \kappa} = \sum_{i=1}^{n} \frac{\partial}{\partial k} (KX_i - Y_i) = \sum_{i=1}^{n} 2 (KX_i - Y_i) \cdot \frac{\partial}{\partial k} (KX_i - Y_i)$  $\Rightarrow$  K =  $32(kx_i-y_i)x_i=0$  $\bigcap$  $\sum_{i=1}^{n} (kx_i - y_i)x_i = 0$  $\sum_{i=1}^{n} (Kx_i^2 - x_iy_i) = 0$  $\sum kx_i^2 - \sum x_i^2 = \sum x_i y_i \longrightarrow K = \frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2}$ 

# 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  $\mathbb{R}^{m \times n}$ .



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

The largest and smallest eigenvalues satisfy

$$
\lambda_{\min}(A) = \inf_{x \neq 0} \frac{x^{\top} A x}{x^{\top} x}, \qquad \lambda_{\max}(A) = \sup_{x \neq 0} \frac{x^{\top} A x}{x^{\top} x}
$$

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

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

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

 $=0 \iff x + y$ <br> $X (2)$  OPTOTOHANGHOCT6 Ecu  $= 0 \le x$  $\langle x,y\rangle$  $Y = \begin{pmatrix} 0 \\ 3 \end{pmatrix}$  $= 2.0 + 0.3=$ Myenno  $x_1 \in \mathbb{R}^n$ ,  $x_2 \in \mathbb{R}^n$ Heieranno X1 ganero ot X2?  $S(x_1, x) = ||x_1 - x_2|| = 0 \leq - \times 1 = x_2$  $\|x\| \geqslant 0$  $\|X\|$  $\|x\| = 0$   $\angle = 0$   $X = 0$  $\left(\begin{matrix} 1 & 0 \\ 0 & 1 \end{matrix}\right)$  $\|\lambda x\| = |\lambda| \cdot \|x\|$  $||x+y|| \le ||x| + ||y||$  $||X^+|| = ||\lambda||^2$ <br> $||X^+|| = \sqrt{\sum_{i=1}^{4} X_i^2}$   $||\lambda|| = \sqrt{\frac{3}{4}}$ Ebraugober  $=5$  $\|X\|_{p} = \left(\sum_{i=1}^{n} |X|^{p}\right)^{\frac{1}{p}}$ 





 $A \succ (\succeq) 0.$ 

The **condition number** of a nonsingular matrix is defined as

 $\kappa(A) = ||A|| ||A^{-1}||$ 

## **Matrix and vector multiplication**

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



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

$$
z = Ax
$$
  
 
$$
\lim_{m \times 1} \lim_{m \times 0} nx \leq
$$

is given by:

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

Finally, just to remind:

$$
C = AB \t CT = BT AT
$$
  
AB \neq BA \t and\n
$$
eA = \sum_{k=0}^{\infty} \frac{1}{k!} Ak
$$

 $e^{A+B} \neq e^{A}e^{B}$  (but if  $A$  and  $B$  are commuting matrices, which means that  $AD = DA$   $A+B = A_0B_1$ 

$$
\frac{AB = BA, e^{-} = e^{-}e^{-} \quad \langle x, y \rangle = \langle x \rangle
$$
\n
$$
\frac{\langle x, Ay \rangle = \langle A^{\top} x, y \rangle}{\langle x' \rangle} = \langle A^{\top} x \rangle \quad \langle x, y \rangle
$$
\nGradient

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



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$$
\nabla f(x) = \frac{df}{dx} = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{pmatrix} \begin{matrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{matrix} + \begin{matrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{matrix} \begin{matrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{matrix} = \begin{matrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_1} \end{matrix} \begin{matrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{matrix} = \begin{matrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_1} \end{matrix} = \begin{matrix} 2x \\ 2y \\ 2z \end{matrix}
$$

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  $x^4$  - HR TO 2kg  $f'(x^*) = 0$ point.  $(x^*)^2 = 0$   $x^* = 0$   $x^* = 0$ 

## **Hessian**

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



In fact, Hessian could be a tensor in such a way:  $(f(x): \mathbb{R}^n \to \mathbb{R}^m)$  is just 3d tensor, 1 of corresponding scalar function<br>
...,  $H(f_m(x)))$ .<br>
10  $(0, 0)$   $(0, 0)$ <br>
10  $(0, 0)$ <br>
10 every slice is just hessian of corresponding scalar function  $(H(f_1(x)), H(f_2(x)), \ldots, H(f_m(x))).$ 

## Jacobian

The extension of the gradient of multidimensional  $f(x): \mathbb{R}^n \to \mathbb{R}^m$  is the following =  $[0.10]$  Msm





∂*f*(*x*) ∂*x*  $\in G$ 

\*



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

\* warpulHo-bekTOpHOe gupaep.

\* SVD, PCA, CNEXTP

 $\lambda(A)$  ,  $\sigma(A)$ 

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

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

Simple derivative

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

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

• *d*(*X*<sup>−</sup>1) = −*X*<sup>−</sup>1(*dX*)*X*<sup>−</sup><sup>1</sup>

# **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 •
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- Online tool for analytic expression of a derivative. •
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