

Lecture 04: Multi-objective optimization

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Often a problem asks us to optimize more than one characteristic of a system. However there are usually trade-offs in doing so; that is, one can optimize a certain trait at the expense of another. For these kinds of problems, there isn't a solution: it's a matter of choice. Today we investigate how to optimize a problem with multiple objectives.

1 Review

Let's review what we've covered in the last couple of lectures considering the equation $Ax = b$ with $A \in \mathbb{R}^{m \times n}$.

Least Squares

- Typically, A is a tall matrix (more equations than variables)
- We would like to find an approximate solution $A\hat{x} \approx b$ as there is typically no x satisfying $Ax = b$ (called the *estimation* setup)
- In optimization notation, the least-squares (LS) problem is written as

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad \|Ax - b\|^2 \quad (1)$$

- The set of solutions of Eq. (1) is precisely the same as the set of solutions to the *normal equations* (2) below.

$$A^T A \hat{x} = A^T b \quad (2)$$

- A solution to the normal equations always exists. That solution is unique if and only if $\text{null}(A) = \{0\}$, i.e. if the columns of A are linearly independent.

Least Norm

- Typically, A is a wide matrix (more variables than equations)
- There are typically infinitely many x satisfying $Ax = b$, so we want to find the “best” x among all solutions (called the *control* setup)
- In optimization notation, the least-norm (LN) problem is written as

$$\begin{aligned} &\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad \|x\|^2 \\ &\text{such that} \quad Ax = b \end{aligned} \quad (3)$$

- The set of solutions of (3) is precisely the same as the set of solutions \hat{x} to the system of equations

$$AA^T w = b \quad \text{and} \quad \hat{x} = A^T w \quad (4)$$

- A solution to Eq. (4) exists if and only if $b \in \text{range}(A)$, i.e. if $Ax = b$ has at least one solution. If a solution exists, it is always unique. Note: there may be many w that solve (4), but they all lead to the same \hat{x} .

2 Defining the Multi-Objective Optimization Problem

Introduction to the cost notation Consider a hybrid version of LS and LN, where we are trying to make both $\|Ax - b\|^2$ and $\|x\|^2$ small at the same time. First, we write these as two separate costs ($J_1 : \mathbb{R}^n \rightarrow \mathbb{R}$ and $J_2 : \mathbb{R}^n \rightarrow \mathbb{R}$). In this case, we have

$$J_1(x) = \|Ax - b\|^2 \quad (5a)$$

$$J_2(x) = \|x\|^2 \quad (5b)$$

Where Equation (5a) above represents the Least Squares problem and Equation (5b) represents the Least norm problem. One can see that a value of x that minimizes one function does not minimize the other. Figure 1 below depicts a 2D plot of $J_1(x)$ and $J_2(x)$ for all the possible x given that A and b are fixed.

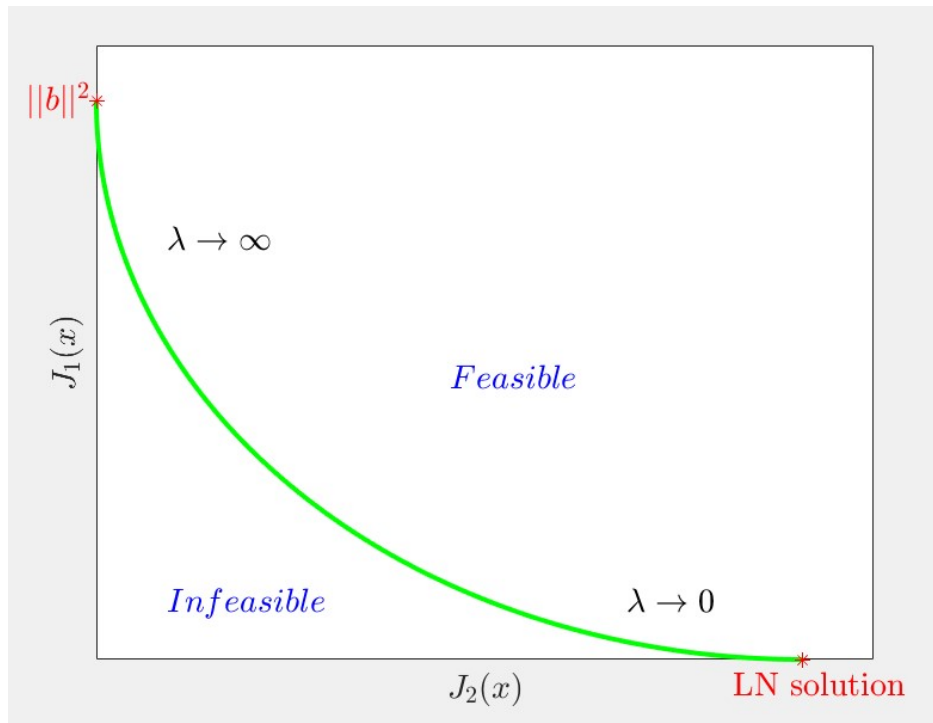


Figure 1: Pareto-optimal front

The green line is the optimal solution, and is called the ‘‘Pareto-optimal front’’. The areas to the right and left of the line are ‘‘feasible’’ and ‘‘infeasible’’, respectively. A natural question may arise from this plot: which point on the line is the best? This question has no answer! Any design on this curve is an optimal solution to the multi-objective problem, and points on the Pareto-optimal front are not comparable unless we assign weights on the objective functions to prioritize them.

A single cost function We can write a single expression that combines these with the help of a weighting parameter $\lambda > 0$ that weights the costs of each accordingly. Eq. (6) below shows that increasing the value of the weight parameter makes the cost function more sensitive to $J_2(x)$, and naturally the converse is true.

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad J_1(x) + \lambda J_2(x) \quad (6)$$

This is actually a least squares problem! Let’s do some manipulation to prove it.

Rearrange into Least Squares problem

1. Substitute Eqs. (5a) and (5b) into Eq. (6).

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad \|Ax - b\|^2 + \|x\|^2 \quad (7)$$

2. Recall block matrix with norm relationship

$$\|x_1\|^2 + \|x_2\|^2 = \left\| \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \right\|^2 \quad (8)$$

3. Rewrite (7) using (8)

$$\|Ax - b\|^2 + \|x\|^2 = \min_x \left\| \begin{bmatrix} Ax - b \\ \sqrt{\lambda}x \end{bmatrix} \right\|^2 \quad (9a)$$

$$= \min_x \left\| \begin{bmatrix} A \\ \sqrt{\lambda}I \end{bmatrix} x - \begin{bmatrix} b \\ 0 \end{bmatrix} \right\|^2 \quad (9b)$$

4. This is a LS problem, so its solution set is the same as that of the normal equations

$$\begin{bmatrix} A \\ \sqrt{\lambda}I \end{bmatrix}^\top \begin{bmatrix} A \\ \sqrt{\lambda}I \end{bmatrix} x = \begin{bmatrix} A \\ \sqrt{\lambda}I \end{bmatrix}^\top \begin{bmatrix} b \\ 0 \end{bmatrix} \quad (10a)$$

$$[A^\top \quad \sqrt{\lambda}I] \begin{bmatrix} A \\ \sqrt{\lambda}I \end{bmatrix} = [A^\top \quad \sqrt{\lambda}I] \begin{bmatrix} b \\ 0 \end{bmatrix} \quad (10b)$$

$$A^\top A + \sqrt{\lambda}I(\sqrt{\lambda}I) = A^\top b + \sqrt{\lambda}I(0) \quad (10c)$$

$$(A^\top A + \lambda I)x = A^\top b \quad (10d)$$

5. The matrix $A^\top A + \lambda I$ is invertible for any $\lambda > 0$ and *any* A .

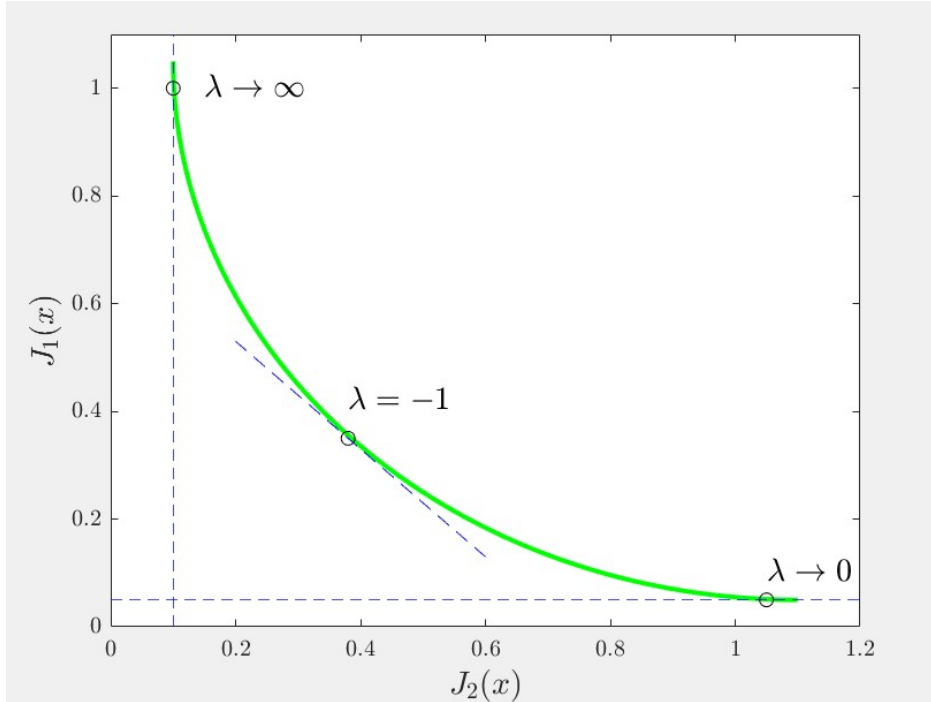


Figure 2: Slope of Pareto-optimal Curve

Geometric interpretation: The trade-off parameter λ is the negative slope of the Pareto-optimal curve. So as we vary $\lambda = 0 \rightarrow \infty$, we start on the bottom-right with a slope of 0 and end on the top-left with a slope of $-\infty$.

3 Special Cases

When $\lambda \rightarrow 0$ in the multi-objective optimization problem, we can recover either the LS or the LN norm solution, depending on the assumptions we make.

LS problem In the LS setting, when $\lambda \rightarrow 0$ and A has full column rank, then $A^T A$ is invertible. Thus, we can take the limit by just setting $\lambda = 0$ and solving (10d).

$$\begin{aligned} \hat{x} &= \lim_{\lambda \rightarrow 0} (A^T A + \lambda I)^{-1} A^T b \\ &= (A^T A)^{-1} A^T b \end{aligned} \tag{11}$$

This is the same solution we found when solving the LS problem in Lecture 2.

LN problem In the LN setting, when $\lambda \rightarrow 0$ and A has full row rank, AA^T is invertible. However, we can't simply set $\lambda = 0$ as we did for LS because $A^T A$ is *not* invertible. We can nevertheless

evaluate the limit using the push-through identity (presented in the next section).

$$\begin{aligned}
 \hat{x} &= \lim_{\lambda \rightarrow 0} (A^T A + \lambda I)^{-1} A^T b \\
 &= \lim_{\lambda \rightarrow 0} A^T (A A^T + \lambda I)^{-1} b \\
 &= A^T (A A^T)^{-1} b
 \end{aligned} \tag{12}$$

This is the same solution we found when solving the LN problem in Lecture 3.

4 The Push-Through Identity

Push-Through Identity: If $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{n \times m}$, then

$$A(BA + \lambda I)^{-1} = (AB + \lambda I)^{-1} A \tag{13}$$

Moreover, $AB + \lambda I$ is invertible if and only if $BA + \lambda I$ is invertible.

Proof:

1. Factor out A from the right and left of $ABA + \lambda A$.

$$\begin{aligned}
 A(BA + \lambda I_n) &= ABA + \lambda A \\
 &= (AB + \lambda I_m)A
 \end{aligned} \tag{14}$$

2. Multiply both sides by $(BA + \lambda I_n)^{-1}$ on the right to isolate A .

$$A = (AB + \lambda I_m)A(BA + \lambda I_n)^{-1} \tag{15}$$

3. Finally, multiply both sides by $(AB + \lambda I_m)^{-1}$ on the left.

$$(AB + \lambda I_m)^{-1}A = A(BA + \lambda I_n)^{-1} \tag{16}$$

Regarding invertibility, suppose $AB + \lambda I$ is *not* invertible. Then there must exist a nonzero element in the nullspace. So there is some $v \neq 0$ such that $ABv + \lambda v = 0$. Multiply both sides by B on the left and obtain $0 = BABv + \lambda Bv = (BA + \lambda I)Bv$. Therefore $Bv \in \text{null}(BA + \lambda I)$. We can't have $Bv = 0$, because then $ABv + \lambda v = \lambda v = 0$, which contradicts the fact that $\lambda > 0$ and $v \neq 0$. Therefore, we have identified a nonzero element of the nullspace of $BA + \lambda I$, which means that $BA + \lambda I$ is not invertible. Applying the same argument starting with $BA + \lambda I$, we conclude that $AB + \lambda I$ is invertible if and only if $BA + \lambda I$ is invertible.

This is called the ‘‘Push-Through’’ identity because in Eq. (13), matrix A is pushed from the left side of $(BA + \lambda I_n)^{-1}$ to the other. Notice in Equation 16, the left hand side requires the inverse of an $m \times m$ matrix while the right hand side requires an inverse of an $n \times n$ matrix. When $m \gg n$ (m much larger than n), this property becomes computationally helpful as we need only compute the inverse of the smaller matrix.



Figure 3: Depiction of mass transfer

5 Revisiting the Mass Transfer Example

We want to move a mass (initially at rest) a distance close to 1 unit in 10 seconds by applying a force every second (time is discretized into 1 second units). First, we start by defining the following variables:

- x_t = position at time t
- v_t = velocity at time t
- f_t = force applied at time t

We will assume that initial conditions are $x_0 = 0$ and $v_0 = 0$ and the dynamics of the system can be described by the following equations

1. $v_{t+1} = v_t + f_t$
2. $x_{t+1} = x_t + v_t$

Goals

1. Make $(x_{10} - 1)^2$ small (get as close to final position as we can)
2. Make $f_0^2 + f_1^2 + \dots + f_9^2$ small (use as little fuel as possible)

Solution Process

First, write all goals in terms of f

$$\begin{aligned}
 x_{10} &= v_0 + v_1 + \dots + v_9 + x_0 \\
 v_1 &= v_0 + f_0 \\
 v_2 &= v_0 + f_0 + f_1 \\
 v_3 &= v_0 + f_0 + f_1 + f_2 \\
 &\vdots \\
 v_{10} &= f_0 + f_1 + f_2 + \dots + f_9
 \end{aligned} \tag{17}$$

Substitute the value for velocity (v_10) into the expression for position(x_10) to yield

$$\begin{aligned}
 x_{10} &= 9f_0 + 8f_1 + 7f_2 + \dots + f_8 \\
 &= [9 \quad 8 \quad 7 \quad \dots \quad 2 \quad 1] \begin{bmatrix} f_0 \\ f_1 \\ \vdots \\ f_8 \end{bmatrix} \\
 &= a^\top f
 \end{aligned} \tag{18}$$

Then write the costs in optimization notation

$$\begin{aligned}
 \mathbf{Goal\ 1:} \quad J_1(f) &= \|a^\top f - 1\|^2 \\
 \mathbf{Goal\ 2:} \quad J_2(f) &= \|f\|^2
 \end{aligned} \tag{19}$$

and then combine them to form a single cost function of the form

$$\min_f \|a^\top f - 1\|^2 + \|f\|^2 \tag{20}$$

and then we solve for \hat{f} using the push through identity

$$\begin{aligned}
 \hat{f} &= (aa^\top + \lambda I)^{-1}a \\
 &= a(a^\top a + \lambda I)^{-1} \\
 &= \frac{1}{\|a\|^2 + \lambda} \cdot a
 \end{aligned} \tag{21}$$

As λ increases (heavily weighting J_2 i.e the cost of fuel) the model would decide not to move and pay the price for not reaching the destination. Conversely, as λ decreases (heavily weighting J_1 i.e distance) the model doesn't care how much fuel is used as long as it ends up in the right place. Fig. 4 below depicts a 2D plot of the trade-off curve (Pareto-optimal front).

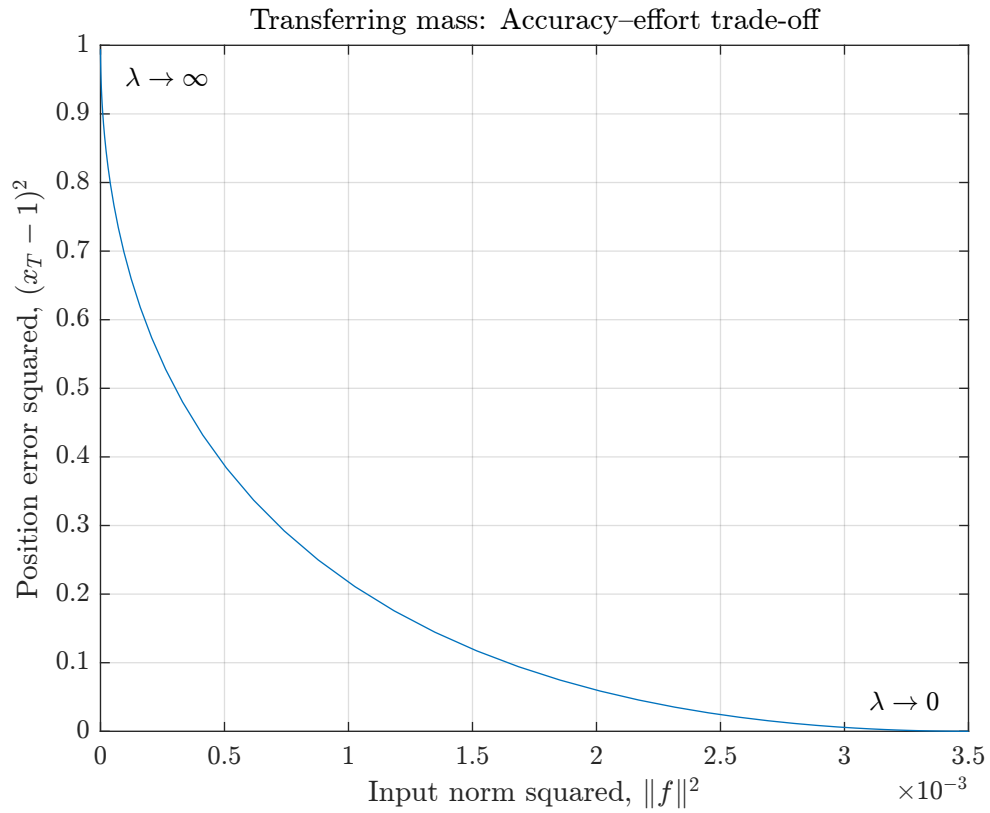


Figure 4: Trade-off curve between the squared position error and the squared norm of the force applied.