MATH60005/70005: Optimisation (Autumn 22-23)

Instructions: read this first!

- This coursework has a total of 20 marks and accounts for 10% of the module.
- Students who want to take the final exam (90%) must submit this coursework.
- **Submission deadline:** Thursday November 24th, 13:00 UK time, via Blackboard drop box.
- Submit a single file, handwritten answers (whenever possible) are allowed but readability is essential and part of the assessment.
- **Marking criteria:** Full marks will be awarded for work that 1) is mathematically correct, 2) shows an understanding of material presented in lectures, 3) gives details of all calculations and reasoning, and 4) is presented in a logical and clear manner.
- Do not discuss your answers publicly via our forum. If you have any queries regarding your interpretation of the questions, please contact the lecturer at dkaliseb@imperial.ac.uk
- Beware of plagiarism regulations. This is an **individual assessment**.

Questions

1. Unconstrained Optimisation.

   i) Construct a function $f : \mathbb{R}^2 \to \mathbb{R}$ which is not coercive and satisfies that for any $\alpha \in \mathbb{R}$

$$\lim_{|x_1|\to\infty} f(x_1, \alpha x_1) = \lim_{|x_2|\to\infty} f(\alpha x_2, x_2) = \infty\,.$$

Solution: we need to construct a function that grows to infinity along lines passing through the origin but which does not blow up through at least one trajectory of any kind. This is satisfied for instance, by

$$f(x_1, x_2) = (x_1 - 1)^2(x_1^2 + x_2^2)$$

In this case

$$\lim_{|x_1|\to\infty} f(x_1, \alpha x_1) = \lim_{|x_1|\to\infty} (x_1 - 1)^2(1 + \alpha^2)x_1^2 = \lim_{|x_2|\to\infty} (\alpha x_2 - 1)^2(1 + \alpha^2)x_2^2 = \infty$$

however, this function is not coercive as $f(1, x_2) = 0$. In general we can consider the product between a coercive function $g(x_1, x_2)$ which will satisfy the limit conditions, and a positive function that vanishes along a trajectory which does not pass through the origin:

$$f(x_1, x_2) = (ax_1 + bx_2 + 1)^2 g(x_1, x_2) \,.$$

Marking rubric: 2 marks for showing the function is non-coercive, 2 marks for having both limits correct.

ii) Find and characterise all the stationary points of:

$$f(x_1, x_2) = 4x_1^4 + x_2^2 - 4x_1^2 x_2 + 4 \,.$$

Solution: The function has the following gradient and Hessian:

$$\nabla f = \begin{pmatrix} 16x_1^3 - 8x_1 x_2 \\ 2x_2 - 4x_1^2 \end{pmatrix}, \qquad \nabla^2 f = \begin{pmatrix} 48x_1^2 - 8x_2 & -8x_1 \\ -8x_1 & 2 \end{pmatrix}$$

From $\nabla f = 0$ it follows that all the stationary points lie along $x_2 = 2x_1^2$, for which the Hessian becomes

$$\nabla^2 f = \begin{pmatrix} 32x_1^2 & -8x_1 \\ -8x_1 & 2 \end{pmatrix}$$

which is positive semidefinite. We also observe that $f(x_1, x_2) = 4x_1^4 + x_2^2 - 4x_1^2 x_2 + 4 = (2x_1^2 - x_2)^2 + 4 \geq 4$, and f at any stationary points reaches the lower bound. Hence, all the stationary points are nonstrict global minimisers.

Marking rubric: 1 mark for finding the stationary points along the curve, 1 mark for showing a local minimizer or 2 marks for concluding a global min.

2. Linear Least Squares.

Consider a dynamical process of the form

$$\begin{aligned} x_0 &= \bar{x} \in \mathbb{R} \,, \\ x_i &= a x_{i-1} + d u_i \,, \quad i = 1, \ldots, N \end{aligned}$$

where $a, d \in \mathbb{R}$. The variables x_i and u_i denote the internal state of the system and a control variable at discrete time i, respectively. The sequence $\mathbf{x}_{\bar{x}}^{\mathbf{u}} := \{x_i\}_{i=0}^N \in \mathbb{R}^{N+1}$ is the trajectory of the system departing from the initial condition $\bar{x}$ associated to the control sequence $\mathbf{u} := \{u_i\}_{i=1}^N \in \mathbb{R}^N$.

Given an initial condition $\bar{x}$, and parameters a, d, and N, our goal is to find an optimal sequence of controls $\mathbf{u}$ which drive the trajectory of the system $\mathbf{x}_{\bar{x}}^{\mathbf{u}}$ to zero while balancing the amount of control energy that is spent in this task. We express our goal as a **dynamic optimisation problem** of the form

$$\min_{\mathbf{u} \in \mathbb{R}^N} \; \|\mathbf{x}\|_2^2 + \frac{\gamma}{2} \|\mathbf{u}\|_2^2 \,, \qquad \gamma > 0 \tag{DO}$$

subject to

$$\begin{aligned} x_0 &= \bar{x} \,, \\ x_i &= a x_{i-1} + b u_i \,, \quad i = 1, \ldots, N. \end{aligned}$$

i) Reformulate (DO) as a regularised linear least squares problem for $\mathbf{u}$. Discuss existence and uniqueness of an optimal solution $\mathbf{u}^*$ to this problem. Show that any $\mathbf{u}$ solving the associated unregularised linear least squares problems (that is, with $\gamma = 0$), satisfies $\|\mathbf{u}^*\| \leq \|\mathbf{u}\|$.
Solution: using the recursion of the discrete dynamics we obtain

$$x_i = ax_{i-1} + bu_i = a(ax_{i-2} + du_{i-1}) = \ldots = a^N x_0 + a^{N-1}du_1 + a^{N-2}du_2 + \ldots + du_N\,.$$

In this way, the trajectory $\mathbf{x}^{\mathbf{u}}_{\bar{x}} := \{x_i\}_{i=0}^N \in \mathbb{R}^{N+1}$ can be represented as $\mathbf{x}^{\mathbf{u}}_{\bar{x}} ::= \mathbf{A}\mathbf{u} - \mathbf{v}$ with

$$\mathbf{A} = d \begin{bmatrix} 1 & & & & & & \\ a & 1 & & & & & \\ a^2 & a & 1 & & & & \\ \vdots & a^2 & a & 1 & & & \\ & \vdots & a^2 & a & 1 & & \\ & & \vdots & a^2 & a & 1 & \\ & & & & & \ddots & \\ a^{N-1} & a^{N-2} & a^{N-3} & \ldots & & & 1 \end{bmatrix}, \quad \mathbf{v} := -\bar{x} \begin{bmatrix} a \\ a^2 \\ a^3 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ a^N \end{bmatrix},$$

such that (DO) can be cast as

$$\min_{\mathbf{u}\in\mathbb{R}^N} \;\|\mathbf{A}\mathbf{u} - \mathbf{v}\|_2^2 + \frac{\gamma}{2}\|\mathbf{u}\|_2^2\,.$$

The matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$ is of full rank, and also $\gamma > 0$, hence the (DO) problem formulated as regularised least squares problem has a unique solution which is given by the normal system

$$(\mathbf{A}^\top\mathbf{A} + \frac{\gamma}{2}\mathbf{I})\mathbf{u}^* = \mathbf{A}^\top\mathbf{v}\,.$$

If we denote by $\mathbf{u}$ a solution to the unregularised problem, that is

$$\min_{\mathbf{u}\in\mathbb{R}^N} \;\|\mathbf{A}\mathbf{u} - \mathbf{v}\|_2^2$$

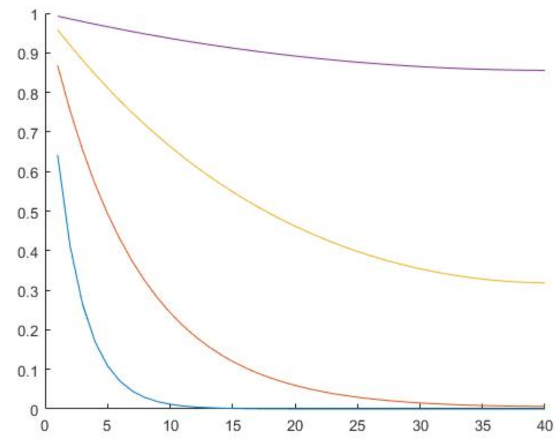
it holds

$$\|\mathbf{A}\mathbf{u}^* - \mathbf{v}\|^2 + \frac{\gamma}{2}\|\mathbf{u}^*\|^2 \leq \|\mathbf{A}\mathbf{u} - \mathbf{v}\|^2 + \frac{\gamma}{2}\|\mathbf{u}\|^2\,,$$

because of the optimality of $\mathbf{u}^*$ for the RLS. From here, it follows from the optimality of $\mathbf{u}$ for the unregularised problem that

$$0 \leq \|\mathbf{A}\mathbf{u}^* - \mathbf{v}\|^2 - \|\mathbf{A}\mathbf{u} - \mathbf{v}\|^2 \leq \frac{\gamma}{2}(\|\mathbf{u}\|^2 - \|\mathbf{u}^*\|^2)\,,$$

leading to $\|\mathbf{u}^*\| \leq \|\mathbf{u}\|$.
Marking rubric: 1 mark for matrix-vector formulations, 1 mark for existence and uniqueness, 2 marks for inequality.



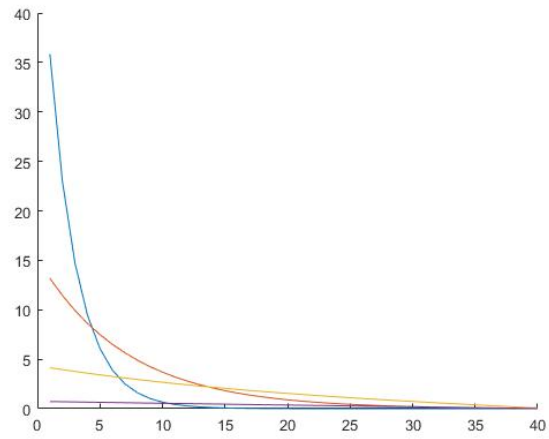


Figure 1: Left: optimal states. Right: optimal controls. As the regularisation parameter γ grows, the control magnitude is reduced, however, this generates an impact on the optimal trajectory, which loses tracking to 0.

ii) For $N = 40$, $a = 1$, $d = -0.01$ and $\bar{x} = 1$, generate two plots, one for the optimal control signals $\mathbf{u}^*$, and another for the associated optimal trajectories $\mathbf{x}_{\bar{x}}^{\mathbf{u}^*}$ for $\gamma = 10^{-3}, 10^{-2}, 0.1, 1$. What is the effect of increasing γ in both the control and the trajectories?

Solution: See Figure 1.

Marking rubric: 1 mark for each plot, 1 mark for discussion.

iii) In many practical applications we want to impose additional bounds on the control signal $\mathbf{u}$. For example, we want to establish an upper bound $u_i \leq u_{max}$ for all i. One way to enforce such a constraint is by using a penalty function, that is, the objective function in (DO) is replaced by

$$\min_{\mathbf{u}\in\mathbb{R}^N} \|\mathbf{x}_{\bar{x}}^{\mathbf{u}}\|_2^2 + \frac{\gamma}{2}\|\mathbf{u}\|_2^2 - \delta \sum_{i=1}^{N} \log(u_{max} - u_i)\,, \qquad \gamma, \delta > 0$$

Generate separate plots for the state and the control when solving the unconstrained problem (as in ii)), for $N = 40$, $a = 1$, $d = -0.01$, $\bar{x} = 1$, $u_{max} = 8$, and $\gamma = \delta = 10^{-2}$. What do you observe? You can use any method discussed in the module, but you need to state your settings.

Solution: because of the logarithmic nonlinearity, the solution of the regularised problem requires an iterative method, in our case this corresponds to gradient descent

$$\mathbf{u}^{k+1} = \mathbf{u}^k - t^k \nabla f(\mathbf{u}^k)\,,$$

where the gradient is given by

$$\nabla f(\mathbf{u}) := 2A^\top(A\mathbf{u} - \mathbf{v}) + \gamma u + \delta \sum_{i=1}^{N} \frac{1}{u_{max} - u_i}\,.$$

Results are presented in Figure 2.

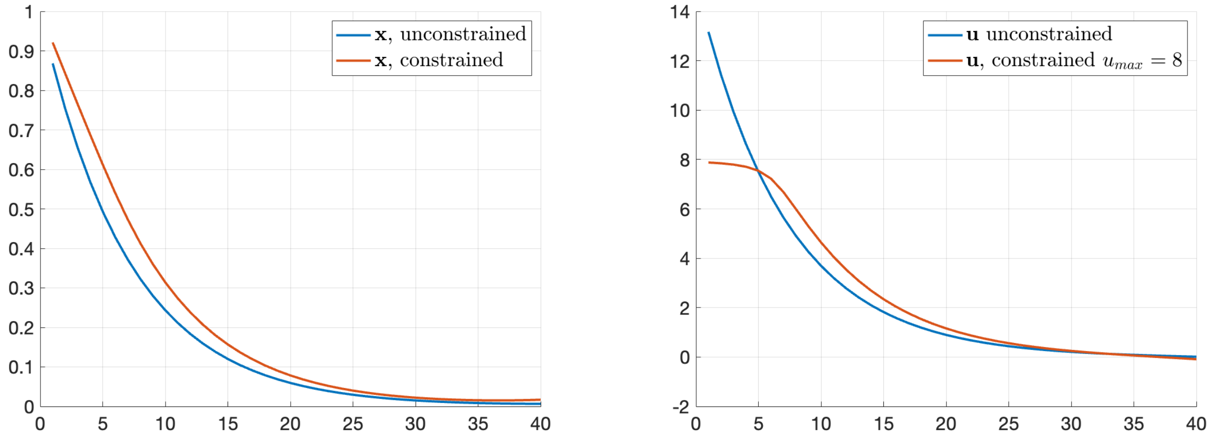


Figure 2: Left: optimal states. Right: optimal controls. In the absence of constraints, we recover the LLS solution. With a logarithmic penalty function, the optimal control is bounded by u_{max}, with a more sustained action in time. The bound impacts the tracking to 0, which is faster and more accurate in the unconstrained case. Results were produced with gradient descent and backtracking $s = 1$, $\alpha = 0.1$, $\beta = 0.9$, and stopping criteria $\|\nabla f\| \leq 10^{-4}$

Marking rubric: 1 mark for each plot, 1 mark for discussion.

iv) As discussed during the lectures, one may also wish to promote sparsity in the control signal $\mathbf{u}$ by considering an ℓ_1 norm penalty in the cost,

$$\min_{\mathbf{u}\in\mathbb{R}^N} \quad \|\mathbf{x}_{\bar{x}}^{\mathbf{u}}\|_2^2 + \frac{\gamma_2}{2}\|\mathbf{u}\|_2^2 + \gamma_1\|\mathbf{u}\|_1\,, \qquad \gamma_1, \gamma_2, \delta > 0\,,$$

however, we haven't discussed yet how to deal with the non-differentiability of the ℓ_1 norm at the origin. Instead, we propose the following approximations to the ℓ_1 norm:

$$\mathcal{L}_\epsilon(\mathbf{u}) := \begin{cases} \frac{1}{2}u_i^2 & \text{if } \ |u_i| \leq \epsilon \\ \epsilon\left(|u_i| - \frac{1}{2}\epsilon\right) & \text{otherwise}\ . \end{cases}$$

Explain in your own words the meaning of the $\mathcal{L}_\epsilon(\mathbf{u})$ as a regulariser, is it a differentiable function? Implement a gradient descent method with backtracking -describe all your settings- to find the optimal solution to

$$\min_{\mathbf{u}\in\mathbb{R}^N} \quad \|\mathbf{x}_{\bar{x}}^{\mathbf{u}}\|_2^2 + \frac{\gamma_2}{2}\|\mathbf{u}\|_2^2 + \gamma_1\mathcal{L}_\epsilon(\mathbf{u})\,, \qquad \gamma_1, \gamma_2, \epsilon > 0\,,$$

and compare the cases

i) $N = 40$, $a = 1$, $d = -0.01$, $\bar{x} = 1$, $\epsilon = 3$, $\gamma_2 = 10^{-2}$, $\gamma_1 = 0\,,$

ii) $N = 40$, $a = 1$, $d = -0.01$, $\bar{x} = 1$, $\epsilon = 3$, $\gamma_2 = 0$, $\gamma_1 = 10^{-2}$.

Solution: this penalty term is called the Huber loss, and close to the origin ($|u_i| \leq \epsilon$) it becomes the ℓ_2 norm, whereas far from the origin it behaves linearly, similar to the ℓ_1 norm. The function is differentiable at $|u_i| = \epsilon$,

$$\frac{\partial \mathcal{L}_\epsilon(\mathbf{u})}{\partial u_i} = \frac{\partial}{\partial u_i}\frac{1}{2}u_i^2 = \frac{\partial}{\partial u_i}\epsilon\left(|u_i| - \frac{1}{2}\epsilon\right) = u_i$$

so, unlike the ℓ_1 norm, and the regularised problem can be computed using gradient descent, with

$$\nabla f(\mathbf{u}) := 2A^\top(A\mathbf{u} - \mathbf{v}) + \gamma_2 u + \gamma_1 \nabla\mathcal{L}_\epsilon(\mathbf{u}), \qquad \nabla\mathcal{L}_\epsilon(\mathbf{u}) := \begin{cases} u_i & \text{if } |u_i| \leq \epsilon \\ \epsilon\frac{u_i}{|u_i|} & \text{otherwise} \end{cases}.$$

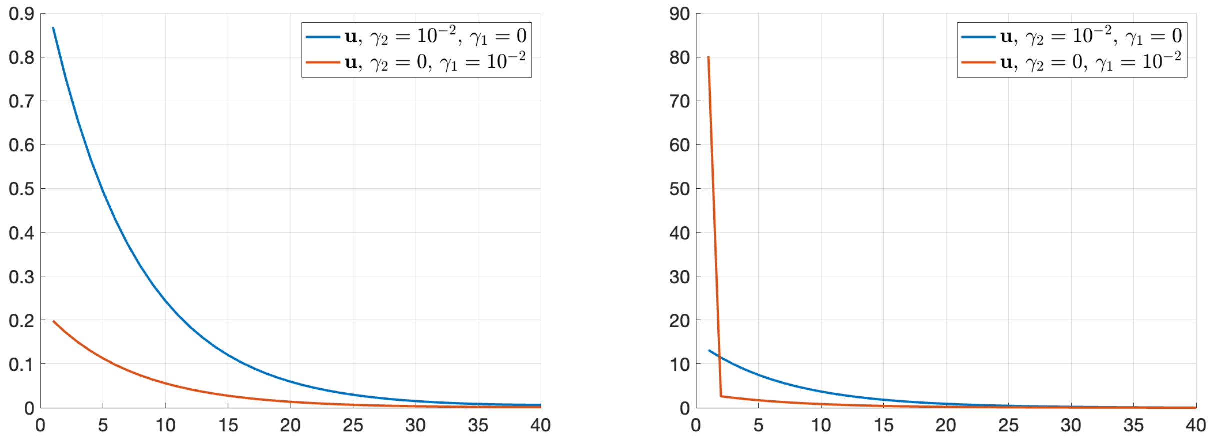


Figure 3: Left: optimal states. Right: optimal controls. The sparsity-promoting regulariser reduces the support of the optimal control, but it increases its magnitude compared to the ℓ_2 control. Such a strong initial control effort is also reflected in the optimal trajectory, which exhibits a faster and more accurate tracking to 0 compared to the ℓ_2 control.

Marking rubric: 1 mark for each plot, 1 mark for discussion (including differentiability).

General feedback

- Q1(i) many students had limits not satisfied for particular values of alpha; some of them tried proving the limits using triangular inequality the wrong way; the function from Q1(ii) satisfied all the requirements.
- Q1(ii) the function is not coercive, not everybody realized that; the most recurrent mistake was to rely only on H positive semidefinite to conclude a global minimizer from that (which is only valid for quadratic functions). Some students analysed the origin as a separate point, although it is part of the stationary curve.
- Q2(i) Some students used a spectral argument for the inequality, but this has to be done carefully because arguments of the type $\|Au\| = \|A\|\|u\|$ were quite common. Many answers took for granted inequalities for matrix norms without giving justification. However, many answers were based in the simpler argument regarding optimality and sub-optimality of the (un)regularised solutions.
- Q2(ii) some students commented the regulariser as if we were dealing with a denoising problem.
- Q2(iii) some students present plots without having a discussion or checking that the initial guess of the constrained solution is feasible.
- Q2(iv) some students didn't plot the optimal trajectories and give differentiability for granted.