Numerical Optimization with Python

Assignment 01 - dry part: Mathematical Review, Optimality Conditions and Convexity

Part 1: Vector differentiation and general preview material

1. Let $a \in \mathbb{R}^n$ a nonzero constant vector and $f: \mathbb{R}^n \to \mathbb{R}$ defined by $f(x) = a^T x$. Use explicit scalar differentiation to show the following:
    a. $\nabla f(x) = a$

Solution:

Since $f(x) = a^T x = \sum_{i=1}^{n} a_i x_i$, differentiating w.r.t x_i gives $\frac{\partial f}{\partial x_i} = a_i$ and hence:

$\nabla f(x) = \left[\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_n}\right]^T = [a_1, \dots, a_n]^T = a$

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    b. $\nabla^2 f(x) = 0 \in \mathbb{R}^{n \times n}$

Solution:

The Hessian is an $n \times n$ matrix, elements of which are $\frac{\partial^2 y}{\partial x_i \partial x_j}$. Since for all i we have that $\frac{\partial f}{\partial x_i} = a_i$ is a constant, any second derivative yields zero, and therefore for all i, j $\frac{\partial^2 y}{\partial x_i \partial x_j} = 0$.

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2. Let $A \in \mathbb{R}^{n\times n}$ by a symmetric matrix and $f: \mathbb{R}^n \to \mathbb{R}$ defined by $f(x) = \frac{1}{2}x^T Ax$. Use explicit scalar differentiation to show the following;
   a. $\nabla f(x) = Ax$

Solution:

First, it is useful to know that $\frac{1}{2}x^T Ax = \frac{1}{2}\sum_{ij} a_{ij}x_i x_j$ (a double summation over both i and j).

This is explained by explicitly working out the multiplication: first Ax has $\sum_{j=1}^{n} a_{ij}x_j$ as its i'th row (note that i is constant here and j is the summation index). Next, we multiplying by x^T gives $\sum_{i=1}^{n} x_i\left[\sum_{j=1}^{n} a_{ij}x_j\right]$. Since i is constant w.r.t to the index of the inner summation:

$$\frac{1}{2}x^T Ax = \frac{1}{2}\sum_{i=1}^{n} x_i\left[\sum_{j=1}^{n} a_{ij}x_j\right] = \frac{1}{2}\sum_{i=1}^{n}\left[\sum_{j=1}^{n} x_i a_{ij}x_j\right] = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}x_i x_j$$

Now we can do the scalar differentiation. We would like to differentiate w.r.t x_k. For $\frac{\partial f}{\partial x_k}$ note that in the above expression $2n-1$ terms are relevant: n terms for which $i = k$ and n for which $j = k$. The case where $i = j = k$ appears once only, and is common to both. If you'd like to easily grasp it, think of the indices of k'th row in a matrix, and then of k'th column in a matrix, and about the fact that they coincide at the diagonal element, index k, k. Any other index has both i and j not equal to k and hence is constant w.r.t x_k and does not appear in the differentiation. We now make it formal:

$$\frac{\partial f}{\partial x_k} = \frac{1}{2}\left[\frac{\partial}{\partial x_k}\left[a_{kk}x_k^2\right] + \frac{\partial}{\partial x_k}\sum_{\substack{j=1,\ldots n\\ j\neq k}} a_{kj}x_k x_j + \frac{\partial}{\partial x_k}\sum_{\substack{i=1,\ldots,n\\ i\neq k}}^{n} a_{ik}x_i x_k\right]$$

$$= \frac{1}{2}\left[\frac{\partial}{\partial x_k}\left[a_{kk}x_k^2\right] + \frac{\partial}{\partial x_k}\left[\sum_{\substack{j=1,\ldots n\\ j\neq k}} a_{kj}x_k x_j + \sum_{\substack{i=1,\ldots n\\ i\neq k}} a_{ik}x_i x_k\right]\right]$$

$$= \frac{1}{2}\left[2a_{kk}x_k + \sum_{\substack{j=1,\ldots n\\ j\neq k}} a_{kj}x_j + \sum_{\substack{i=1,\ldots n\\ i\neq k}} a_{ik}x_i\right] = \frac{1}{2}\left[\sum_{j=1}^{n} a_{kj}x_j + \sum_{i=1}^{n} a_{ik}x_i\right]$$

The first sum is exactly row k of A multiplied by the column vector x. The second sum is exactly column k of A (and hence it is row k of A^T) multiplied by the column vector x. Put together, we have shown that: $\nabla f(x) = \frac{1}{2}[A + A^T]x$.

This was worth noting, and the fact that A is symmetric was intentionally ignored up until this stage. Finally, as in the question A is symmetric, we can continue:

$$\nabla f(x) = \frac{1}{2}[A + A^T]x = \frac{1}{2}[A + A]x = Ax$$

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b. $\nabla^2 f(x) = A$

Solution:

For $\nabla^2 f(x)$ we need the Differential matrix (also referred to as the Jacobian matrix) of the vector valued mapping $x \mapsto Ax$. Well, this is a linear map and its differential is simply A. However, we required explicit scalar differentiation.

As reviewed in the preview material in the first class (see the slides of Lecture 01), the differential matrix Dg of a mapping $g: \mathbb{R}^n \to \mathbb{R}^d$is the matrix of all partial derivatives of first order: $[Dg]_{ij} = \frac{\partial g_i}{\partial x_j}$ (each row is a gradient of a scalar component of the vector valued mapping, as a row vector). Since in part (a) of the question we have shown that gradient of $x \mapsto a^T x$ is a, and since each scalar component of $x \mapsto Ax$ is $a_i x$ where a_i is row i of A, we conclude that indeed, as expected, A is the differential matrix.

We now apply it to the question. Since $\nabla f(x) = \frac{1}{2}[A + A^T]x$, we have that

$\nabla^2 f(x) = \frac{1}{2}[A + A^T]$, and again in the symmetric case, this is exactly A.

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3. Given a twice differentiable function $f: \mathbb{R}^n \to \mathbb{R}$, use the chain rule to show how ∇f and $\nabla^2 f$ are modified under an affine change of variable $z = Ax + b$, namely define $g(x) = f\big(z(x)\big)$ and express $\nabla g(x), \nabla^2 g(x)$ using ∇f and $\nabla^2 f$.

Solution:

To solve this question we simply need the chain rule, but we must also review the following (see the chain rule in the preview material slides of Lecture 01):

1. The chain rule in its general form for vector valued mappings.
2. The subtle difference between the row vector of partial derivatives (the differential of a scalar valued function, which we view as a linear functional operating by row-column multiplication), and the gradient, which by convention is just the column vector with the same elements.

Define $g(x) = f(Ax + b)$. We use the chain rule in its general form for mappings, where the composition of maps is differentiated as the matrix multiplication of the differential matrices. Differentiating:

$$Dg(x) = Df(Ax + b)Dz(x) = Df(z)A$$

So far this was the chain rule, working with differential matrices: differential matrices are linear operators for which the dimensions of the matrix multiplication are well defined and work (for scalar valued functions the differentials are row vectors of partial derivatives).

Note that this gave us a row vector, and recall that our convention is that ∇f denotes the column vector, which is the transpose of the corresponding single row differential matrix, and therefore the required form of the answer is:

$$\nabla g(x) = [Df(z)A]^T = A^T[Df(z)]^T = A^T \nabla f(z)$$

To continue and answer for $\nabla^2 g$, we need the differential matrix of ∇g. Again we use the chain rule, and also the basic vector differentiation rules from the previous questions:

$$D[A^T \nabla f(z)] = A^T \nabla^2 f(z) A$$

Note that in this case, we do not worry about transposing because the result is symmetric

(assuming $f \in C^2$)

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4. Let $a \in \mathbb{R}^n$ be a constant, nonzero vector and $b \in \mathbb{R}$. What is the distance of a point $p \in \mathbb{R}^n$ from the hyper-plane $a^T x = b$?

Solution:

The distance from p to the hyper-plane is the distance from p to a point p_0 on the hyper-plane, such that $p - p_0$ is orthogonal to the hyper-plane. Since $\frac{a}{\|a\|}$ is the unit normal vector to the hyper-plane, we know there is some scalar λ such that $p - p_0 = \lambda \frac{a}{\|a\|}$, and that the distance we are seeking is $|\lambda|$. Now, multiplying both sides by a^T gives:

$$a^T(p - p_0) = \frac{\lambda}{\|a\|} a^T a$$

As for the LHS, we have: $a^T p - a^T p_0 = a^T p - b$ since p_0 belongs to the hyper-plane. For the RHS, remember that $a^T a = \|a\|^2$ and hence:

$$a^T p - b = \lambda \|a\|$$

And the distance we seek is:

$$|\lambda| = \left| \frac{a^T p - b}{\|a\|} \right|$$

Part 2: Optimality conditions for unconstrained optimization

1. Consider $f(x_1, x_2) = 8x_1 + 12x_2 + x_1^2 - 2x_2^2$.
    a. Write f in vector form, that is: represent $f(x) = x^T Q x + q^T x + c$ for appropriate matrix, vector and scalar Q, q and c, respectively.

Solution:

Either by inspection or from explicitly working out the multiplication, we arrive at:

$$f(x_1, x_2) = 8x_1 + 12x_2 + x_1^2 - 2x_2^2 = [x_1, x_2]\begin{bmatrix}1 & 0\\ 0 & -2\end{bmatrix}\begin{bmatrix}x_1\\ x_2\end{bmatrix} + [8,12]\begin{bmatrix}x_1\\ x_2\end{bmatrix}$$

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b. Show that f has only one stationary point, and that it is neither a max nor a min, but a saddle.

Solution:

By now we have proven all the required vector differentiation formulas we need, thus we do not differentiate each scalar component but use the vector differentiation we already know:

$$\nabla f(x_1, x_2) = 2\begin{bmatrix}1 & 0\\ 0 & -2\end{bmatrix}\begin{bmatrix}x_1\\ x_2\end{bmatrix} + \begin{bmatrix}8\\ 12\end{bmatrix} = \begin{bmatrix}2x_1 + 8\\ -4x_2 + 12\end{bmatrix}$$

This gradient vanishes only at $\begin{bmatrix}-4\\ 3\end{bmatrix}$, indeed a unique stationary point. This point is not a max or a min but a saddle, since the Hessian (a constant matrix in this case) is $2\begin{bmatrix}1 & 0\\ 0 & -2\end{bmatrix}$, and this matrix is sign-indefinite: eigenvalues are $2, -4$ namely there are directions of positive curvature and directions of negative curvature.

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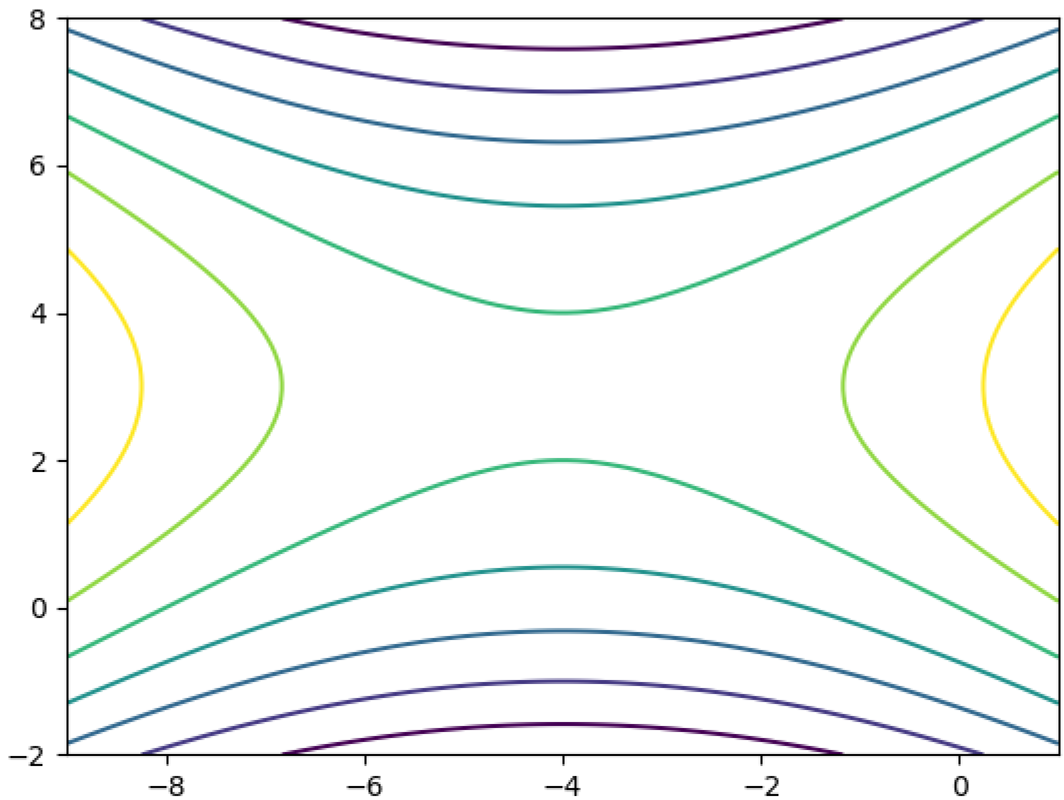
c. Provide a rough sketch of the contour lines of f.

Solution:

The following sketch is obtained with Python in the same way you were required for the programming part of this exercise. Indeed the saddle point is at the expected location:



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2. Define the Rosenbrock function: $f(x) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$.
   a. Compute $\nabla f(x)$ and $\nabla^2 f(x)$

Solution:

Here we work out the answer by straight forward differentiation:

$$\nabla f(x_1, x_2) = \begin{bmatrix} 200(x_2 - x_1^2)(-2x_1) - 2(1 - x_1) \\ 200(x_2 - x_1^2) \end{bmatrix} = \begin{bmatrix} -400(x_1x_2 - x_1^3) - 2(1 - x_1) \\ 200(x_2 - x_1^2) \end{bmatrix}$$

$$\nabla^2 f(x_1, x_2) = \begin{bmatrix} -400x_2 + 1200x_1^2 + 2 & -400x_1 \\ -400x_1 & 200 \end{bmatrix}$$

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b. Show that $x^* = (1,1)^T$ is the only local minimizer of f, and that the Hessian is positive definite at that point.

Solution:

To find a stationary point we first look at $\frac{\partial f}{\partial x_2} = 200(x_2 - x_1^2)$. To vanish we must have:

$x_2 - x_1^2 = 0 \Rightarrow x_2 = x_1^2$. Substituting this into $\frac{\partial f}{\partial x_2} = -400(x_1 x_2 - x_1^3) - 2(1 - x_1)$ we obtain: $-400(x_1^3 - x_1^3) - 2(1 - x_1)$ and requiring this to vanish means $x_1 = 1$. Therefore $x_2 = 1^2 = 1$ and the only stationary point is $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$.

Evaluating the Hessian at this point gives:

$$\nabla^2 f(1,1) = \begin{bmatrix} -400 + 1200 + 2 & -400 \\ -400 & 200 \end{bmatrix} = \begin{bmatrix} 802 & -400 \\ -400 & 200 \end{bmatrix}$$

This matrix is positive definite, as all its leading principal minors are positive, as they are 802 and $802 \times 200 - (-400) \times (-400) = 400$

Summarizing, we found a unique stationary point and a positive definite Hessian, hence it is a local minimizer, and the only one.

Part 3: Convex sets and convex functions

1. Prove that the intersection of convex sets is convex.

   Proof:

   Let $A, B \subseteq \mathbb{R}^n$ be convex sets and let $x, y \in A \cap B$. Consider $z = \alpha x + (1 - \alpha)y$ for some $\alpha \in [0,1]$. Since $x, y \in A$ and A convex, $z \in A$. Since $x, y \in B$ and B convex, $z \in B$. This means $z \in A \cap B$ and therefore $A \cap B$ is convex.

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2. The *sum of two sets* A, B is defined as follows: $A + B := \{a + b : a \in A, b \in B\}$. Prove that the sum of convex sets is a convex set.

Proof:

Denote $C = A + B$, and let $x, y \in C$. Consider $z = \alpha x + (1 - \alpha)y$ for some $\alpha \in [0,1]$.
Since $x, y \in C$ there are $x_a, y_a \in A$ and $x_b, y_b \in B$ such that $x = x_a + x_b$ and $y = y_a + y_b$.
From convexity of A we know that $\alpha x_a + (1 - \alpha)y_a \in A$, and from convexity of B we know that $\alpha x_b + (1 - \alpha)y_b \in B$.
Now, $z = \alpha x + (1 - \alpha)y = \alpha x_a + \alpha x_b + (1 - \alpha)y_a + (1 - \alpha)y_b = \alpha x_a + (1 - \alpha)y_a + \alpha x_b + (1 - \alpha)y_b = [\alpha x_a + (1 - \alpha)y_a] + [\alpha x_b + (1 - \alpha)y_b]$
We have found a representation of z as a sum of a point in A and a point in B, and therefore $z \in A + B$ and hence $A + B$ is convex.

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3. The set Y is *an affine transformation of a set* X, if it is simply the set of all affine transformations of elements of X, namely: $Y = \{Ax + b : x \in X\}$ where A, b are a constant matrix and vector of the appropriate dimensions. Prove that affine transformations of convex sets are convex sets.

Proof:

Assume Y is an affine transformation of the convex set X, with matrix A and vector b. Choose $u, v \in Y$. Denote $w = \alpha u + (1 - \alpha)v$ for some $\alpha \in [0,1]$. Since $u \in Y$, there is $x_u \in X$ such that:

$$u = Ax_u + b$$

Similarly for v we have a representation:

$$v = Ax_v + b$$

To find such representation for w:

$$w = \alpha u + (1 - \alpha)v = \alpha[Ax_u + b] + (1 - \alpha)[Ax_v + b] = A[\alpha x_u + (1 - \alpha)x_v] + b$$

This is indeed the required representation, since by convexity of X, $\alpha x_u + (1 - \alpha)x_v \in X$ and hence Y is convex.

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4. If $\|\cdot\|$ is any norm (not necessarily Euclidean) then any ball: $B(x_0, r) = \{x: \|x - x_0\| \leq r\}$ is a convex set (hint: apply the properties of norms. It may also be convenient to prove for the origin and then use part 3).

Proof:

Due to q. 3, it suffices to show for $B(0, r)$, now denoted B. Choose $u, v \in B$. Denote

$w = \alpha u + (1 - \alpha)v$ for some $\alpha \in [0,1]$. We need to show that $w \in B$, namely that $\|w\| \leq r$. Indeed:

$$\|w\| = \|\alpha u + (1 - \alpha)v\| \leq \|\alpha u\| + \|(1 - \alpha)v\| = |\alpha|\|u\| + |(1 - \alpha)|\|v\|$$
$$= \alpha\|u\| + (1 - \alpha)\|v\| \leq \alpha r + (1 - \alpha)r = r$$

For the first inequality we have used the triangle inequality, then we used he homogeneous property of norms, then the fact that α and $1 - \alpha$ are non-negative, and finally we used the fact that $u, v \in B$. The same arguments hold for an open ball, as the last inequality will become strict and the proof also holds for strict inequality.

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5. Prove that the solutions of a set of linear equalities and inequalities is a convex set.

Proof:

First, linear spaces are convex, since they are closed under linear combinations and therefore under convex combinations. Solutions of linear equations are affine sub-spaces, which are just translations of linear spaces, and by q. 3 translation preserves convexity.

As for solutions of linear inequalities, these are half-spaces, which are also convex. To see this, let $a^T x \leq b$ be a half space denoted H, and let $u, v \in H$. Denote $w = \alpha u + (1 - \alpha)v$ for some $\alpha \in [0,1]$. To check that $w \in H$:

$$a^T w = a^T(\alpha u + (1 - \alpha)v) = \alpha a^T + (1 - \alpha)a^T v \leq \alpha b + (1 - \alpha)b = b$$

We have used the non-negativity of $\alpha, 1 - \alpha$ in the inequality, and the fact that $u, v \in H$.

We have shown that the solution set of a single equality or a single inequality is convex. The solution to many of them is thus the intersection of convex sets, which is convex (as shown in q1).

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6. Let f, g be convex functions. Prove that $\alpha f + \beta g$ is a convex function, non-negative scalars α, β.

Proof:

The domain of $\alpha f + \beta g$ is the intersection of both domains and hence a convex set.

Consider $x, y \in \mathrm{dom} f \cap \mathrm{dom} g$ and $t \in [0,1]$. From convexity of f, g we have:

$$f(tx + (1-t)y) \leq tf(x) + (1-t)f(y)$$

$$g(tx + (1-t)y) \leq tg(x) + (1-t)g(y)$$

To show the convexity of $\alpha f + \beta g$:

$$\begin{aligned}(\alpha f + \beta g)(tx + (1-t)y) &= \alpha f(tx + (1-t)y) + \beta g(tx + (1-t)y) \\ &\leq \alpha[tf(x) + (1-t)f(y)] + \beta[tg(x) + (1-t)g(y)] \\ &= t(\alpha f + \beta g)(x) + (1-t)(\alpha f + \beta g)(y)\end{aligned}$$

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7. Pointwise max: Let f, g be convex functions. Prove that $h(x) := \max\{f(x), g(x)\}$ is a convex function.

Proof:

We need some simple properties of taking the max of two numbers.

a) $a \leq c, b \leq d \Rightarrow \max(a, b) \leq \max(c, d)$. This can be verified by simple case analysis, whoever the winner is in the LHS, the winner on the RHS is at least as strong.

b) $\alpha \geq 0 \Rightarrow \max(\alpha x, \alpha y) = \alpha \max(x, y)$. This is understood again by simply checking the two possible cases.

c) $\max(a + b, c + d) \leq \max(a, c) + \max(b, d)$. To see this, observe that LHS is the max of a specific pair, which is realized by the RHS but the RHS has more potential pairs as candidates.

Now choose u, v in the common domain and $\alpha \in [0,1]$. We use all the above properties in the following chain of inequalities and equalities, along with the convexity of f, g, and show the required inequality for the definition of convexity of h:

$$h(\alpha u + (1-\alpha)v) = \max[f(\alpha u + (1-\alpha)v), g(\alpha u + (1-\alpha)v)]$$
$$\le \max[\alpha f(u) + (1-\alpha)f(v), \alpha g(u) + (1-\alpha)g(v)\,] \le \max[\alpha f(u), \alpha g(u)]$$
$$+ \max[(1-\alpha)f(v), (1-\alpha)g(v)\,]$$
$$= \alpha \max[f(u), g(u)] + (1-\alpha)\max[f(v), g(v)] = \alpha h(u) + (1-\alpha)h(v)$$

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8. A sub-level set of a function $f: \mathcal{D} \subset \mathbb{R}^n \to \mathbb{R}$ is defined as follows: $\{x \in \mathcal{D}: f(x) \le c\}$ where c is a constant scalar. Prove that sub-level sets of convex functions are convex sets.

Proof:

Assume u, v in the sub level set $S = \{x \in \mathcal{D}: f(x) \le c\}$. Denote $w = \alpha u + (1-\alpha)v$ for some $\alpha \in [0,1]$. To show that $w \in S$ we must show that $f(w) \le c$. Indeed:

$$f(w) = f(\alpha u + (1-\alpha)v\,) \le \alpha f(u) + (1-\alpha)f(v) \le \alpha c + (1-\alpha)c = c$$

Where in the first inequality we have used the convexity of f, and in the second inequality we have used the non-negativity of $\alpha, 1-\alpha$ and the fact that $u, v \in S$.

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9. Composition: let $g: \mathcal{D} \subset \mathbb{R}^n \to \mathbb{R}$ be a convex function and let $h: \mathbb{R} \to \mathbb{R}$ be convex and monotone increasing. Prove that $h \circ g: \mathcal{D} \subset \mathbb{R}^n \to \mathbb{R}$ is convex. Provide a counter example if we drop only the monotonic requirement on h. Provide another counter example if we drop only the convexity requirement on h.

Solution:

To prove $h \circ g$ is convex first observe that its domain is convex as it is defined over $\mathcal{D}$. Now, for $u, v \in \mathcal{D}$ and $\alpha \in [0,1]$, we know from convexity of g that:

$$g(\alpha u + (1-\alpha)v) \le \alpha g(u) + (1-\alpha)g(v)$$

From the monotone increasing property of h we know that $t_1 > t_2 \Rightarrow h(t_1) \geq h(t_2)$. Combining the above we so far can write that:

$$h \circ g(\alpha u + (1-\alpha)v) \leq h\big(\alpha g(u) + (1-\alpha)g(v)\big)$$

Now, from convexity of h, the RHS expression also satisfies:

$$h\big(\alpha g(u) + (1-\alpha)g(v)\big) \leq \alpha h \circ g(u) + (1-\alpha)h \circ g(v)$$

which means $h \circ g(\alpha u + (1-\alpha)v) \leq \alpha h \circ g(u) + (1-\alpha)h \circ g(v)$ as required.

Now assume we drop the monotonic increasing requirement. Define $g(x) = x^2$ and $h(y) = -y$. Then, all conditions are met except that h is not monotone increasing. Indeed $h \circ g(x) = -x^2$ is not convex.

Finally, assume we drop the convexity assumption on h. Define $g(x) = x$ which is convex, and $h(y) = \log y$ which is monotone increasing but not convex. Then $h \circ g(x) = \log x$ which is indeed not convex, as required.