

A APPENDIX

A.1 Proof of Lemma A.1

We first prove the following helpful lemma:

LEMMA A.1. *Let $f(x) : \mathbb{R}^m \rightarrow \mathbb{R}$ be twice differentiable $x \in \mathbb{R}^m$. If $Hessian(f, x)$ is indetermimant then so is $Hessian(-f, x)$*

PROOF. If $Hessian(f, x)$ is indetermimant then it has both positive and negative eigenvalues. The eigenvalues of $Hessian(-f, x)$ will just be -1 times each eigenvalue of $Hessian(f, x)$, hence there will still be both positive and negative eigenvalues meaning $Hessian(-f, x)$ is indetermimant. \square

A.2 Full Chain Rule Proof for Intervals

The correctness of the interval bounds also follows nearly identically as the proof for zonotopes, albeit there is a single edge case whenever $\exists x^* \in [l_x, u_x] : f''(x^*) = 0$ and $f'(x^*) = 0$ as the Hessian test would be inconclusive (since its determinant would be 0), but unlike with zonotopes, we cannot ensure that the gradient at x^* is non-zero (as we did by enforcing $A \neq 0$) since there could be x^* such that both $f'(x^*) = f''(x^*) = 0$. If the function f is such that there is never any shared root of both f' and f'' , the proof is complete as this will never happen (this is the case for $\exp, \log, \sigma, \tanh$) but for functions like x^4 or x^3 it is possibility. However any such x^* will be a root of $f''(x) \cdot y$ for any value of y , hence we can call the same verified root solver with $A = 0, y = l_y$ to obtain the x^* . Further, $f'(x^*) = f''(x^*) = 0$ implies $f'(x^*) \cdot y = 0$ for all y , hence checking at (x^*, l_y) is sufficient, and this point is already included in the points we evaluate.

A.3 Full Product Rule Proof for Intervals

Unlike in the case of the Chain rule where some of the cases depended on ensuring the gradients were nonzero, which had to be handled differently for zonotopes vs. intervals, the entire technique for product rule relies only on the Hessian information which will be the same for intervals in order to compute $\min(x_1 \cdot y_2) + (x_2 \cdot y_1)$ and $\max(x_1 \cdot y_2) + (x_2 \cdot y_1)$ since $Hessian((x_1 \cdot y_2) + (x_2 \cdot y_1) - (Ax_1 + By_1 + Cx_2 + Dy_2 + E))$ is the same as $Hessian((x_1 \cdot y_2) + (x_2 \cdot y_1))$. Thus for computing the bounds on the zonotope error symbol and computing the precise interval lower and upper bounds, it suffices to simply check the 2^4 corners.

A.4 Full Quotient Rule Proof for Zonotopes

Having proven that the 4D Hessian is indetermimant at every point, this ensures that the optimal values must occur on the boundaries. We will repeat this idea for the lower dimensional subproblems and show that when restricted to the 3 dimensional boundaries, they also do not have any interior extrema, thus the optimal value must occur on *their* boundaries (the boundary of the boundaries of the 4-cube).

We now detail the rest of the cases for the quotient rule for the Zonotope case

A.4.1 3D Subproblems.

PROOF. Case 1) Fixed y_2 to either l_{y_2} or u_{y_2} - we denote the fixed constant value of y_2 as κ_{y_2} , hence $\kappa_{y_2} \in \{l_{y_2}, u_{y_2}\}$. In this case the first derivatives are:

$$\begin{aligned} \frac{\partial}{\partial x_1} &= \frac{\kappa_{y_2}}{x_2^2} - A \\ \frac{\partial}{\partial y_1} &= \frac{1}{x_2} - B \end{aligned}$$

$$\frac{\partial}{\partial x_2} = \frac{2x_1\kappa_{y_2} - y_1x_2}{x_2^3} - C$$

If $\kappa_{y_2} = 0$, then $\frac{\partial}{\partial x_1} \neq 0$ since by requirement $A \neq 0$, and $x_2 \neq 0$, thus there is no critical point since the gradient $(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial y_1}, \frac{\partial}{\partial x_2})$ cannot be the all-zeros vector.

If $\kappa_{y_2} \neq 0$ then because $x_2 \neq 0$, $A, B \neq 0$, we can ensure that $\frac{\partial}{\partial x_1} \neq 0$ by requiring the condition on A, B that $\frac{A}{B^2} \neq \kappa_{y_2}$. Since for any $x_2 \in [l_{x_2}, u_{x_2}]$ this guarantees that $\frac{\kappa_{y_2}}{x_2^2} - A$ and $\frac{1}{x_2} - B$ cannot both be zero. Thus why we require both $\frac{A}{B^2} \neq l_{y_2}$ and $\frac{A}{B^2} \neq u_{y_2}$.

Case 2) Fixed x_2 to either l_{x_2} or u_{x_2} - we denote the fixed constant value of x_2 as κ_{x_2} . In this case the first derivatives are:

$$\begin{aligned}\frac{\partial}{\partial x_1} &= \frac{y_2}{\kappa_{x_2}^2} - A \\ \frac{\partial}{\partial y_1} &= \frac{1}{\kappa_{x_2}} - B \\ \frac{\partial}{\partial y_2} &= \frac{x_1}{\kappa_{x_2}^2} - D\end{aligned}$$

It suffices to require that $\frac{1}{B} \neq \kappa_{x_2}$, as this guarantees that $\frac{\partial}{\partial y_1} \neq 0$, thus the gradient cannot be the all-zeros vector.

Case 3) Fixed y_1 to either l_{y_1} or u_{y_1} - we denote the fixed constant value of y_1 as κ_{y_1} , hence $\kappa_{y_1} \in \{l_{y_1}, u_{y_1}\}$. In this case the first derivatives are:

$$\begin{aligned}\frac{\partial}{\partial x_1} &= \frac{-y_2}{x_2^2} - A \\ \frac{\partial}{\partial x_2} &= \frac{2x_1y_2 - \kappa_{y_1}x_2}{x_2^3} - C \\ \frac{\partial}{\partial y_2} &= \frac{-x_1}{x_2^2} - D\end{aligned}$$

For this case we will show that any hypothetical root of the above system of equations (which is what is needed for a critical point) is necessarily a saddle point.

Case 3.1) $\kappa_{y_1} \neq 0$. If $\frac{\partial}{\partial x_1} = \frac{\partial}{\partial x_2} = \frac{\partial}{\partial y_2} = 0$ then any critical point will be a root of the above system of equations, furthermore such a root (x_1^*, x_2^*, y_2^*) would be of the form: $(-Dx_2^{*2}, x_2^*, -Ax_2^{*2})$, as that would be needed to ensure that $\frac{\partial}{\partial x_1} = \frac{\partial}{\partial y_2} = 0$. Plugging such a hypothetical root into $\frac{\partial}{\partial x_2} = 0$ implies that x_2^* must *also* be a root of

$$\frac{2ADx_2^{*4} - \kappa_{y_1}x_2^*}{x_2^{*3}} - C = 0$$

But since x_2^* must be nonzero, then equivalently it must be a root of:

$$x_2^{*3} - \frac{C}{2AD}x_2^{*2} - \frac{\kappa_{y_1}}{2AD} = 0$$

Furthermore the Hessian determinant is $-\frac{2(x_1y_2 + \kappa_{y_1}x_2)}{x_2^5}$, however the Hessian has 0 in its upper left corner, meaning the Hessian is neither positive definite nor negative definite (Sylvester's criteria). Thus if the Hessian determinant is non-zero, then the Hessian is necessarily indeterminate meaning the hypothetical root would be a saddle point. Thus we simply need to show that at

such a hypothetical root $(-Dx_2^{*2}, x_2^*, -Ax_2^{*2})$, the Hessian determinant is non-zero. The Hessian determinant is non-zero provided that the numerator $(x_1y_2 + \kappa_{y_1}x_2) \neq 0$, However computing this numerator at our hypothetical root gives:

$$(AD(x_2^*)^4 + \kappa_{y_1}x_2^*)$$

Which is zero if $x_2^* = 0$ (which is not possible) or:

$$x_2^* = \sqrt[3]{\frac{-\kappa_{y_1}}{AD}}$$

Thus we just need to ensure that $\sqrt[3]{\frac{-\kappa_{y_1}}{AD}}$ is not also a root of $x_2^{*3} - \frac{C}{2AD}x_2^{*2} - \frac{\kappa_{y_1}}{2AD} = 0$. We can ensure this by requiring that

$$\sqrt[3]{\frac{-\kappa_{y_1}}{AD}} \neq \frac{-3\kappa_{y_1}}{2C}$$

Case 3.2) $\kappa_{y_1} = 0$. In this case it is still true that any root would be of the form $(-Dx_2^{*2}, x_2^*, -Ax_2^{*2})$, further because $\kappa_{y_1} = 0$, x_2^* must necessarily be

$$x_2^* = \frac{C}{2AD}$$

However, as before the Hessian has a 0 in the upper left corner meaning it is not positive definite or negative definite, furthermore the determinant is $-\frac{2x_1y_2}{x_2^8}$, which at the point $(-D(\frac{C}{2AD})^2, \frac{C}{2AD}, -A(\frac{C}{2AD})^2)$ is non-zero meaning the Hessian is indeterminate

It is worth noting that the Reverse mode version of the quotient rule is an instance of this case.

Case 4) Fixed x_1 to either l_{x_1} or u_{x_1} - we denote the fixed constant value of x_1 as κ_{x_1} . In this case the first derivatives are:

$$\begin{aligned} \frac{\partial}{\partial y_1} &= \frac{1}{x_2} - B \\ \frac{\partial}{\partial x_2} &= \frac{2\kappa_{x_1}y_2 - y_1x_2}{x_2^3} - C \\ \frac{\partial}{\partial y_2} &= \frac{\kappa_{x_1}}{x_2^2} - D \end{aligned}$$

If $\kappa_{x_1} = 0$, then $\frac{\partial}{\partial y_2} = -D$ and $D \neq 0$, hence it is impossible for there to be an extrema. If $\kappa_{x_1} \neq 0$, then it suffices to require that $\kappa_{x_1} \neq \frac{-D}{A^2}$. This is because $\frac{1}{x_2} - B = 0 = \frac{\kappa_{x_1}}{x_2^2} - D$ implies that $B^2 = \frac{-D}{\kappa_{x_1}}$. Hence by the contrapositive $\frac{1}{x_2} - B = 0 = \frac{\kappa_{x_1}}{x_2^2} - D$ cannot have been true. \square

A.4.2 2D Subproblems. Here we show that when solving for the optimal values along the boundary of the boundary, we can still ensure that there are no interior critical points, and thus all local extrema must occur on the boundary of the boundary of the boundary.

PROOF. Case 1) Fixed x_2, y_2 to κ_{x_2} and κ_{y_2} respectively. In this case the function $\frac{(x_2 \cdot y_1) - (x_1 \cdot y_2)}{x_2^2} - (Ax_1 + By_1 + Cx_2 + Dy_2 + E)$ becomes linear in both dimensions, and the optimal values will occur at the corner points and hence there are no interior critical points.

Case 2) Fixed y_1, y_2 to κ_{y_1} and κ_{y_2} respectively. The 2D Hessian determinant in this 2D subproblem is $\frac{-4\kappa_{y_2}^2}{x_2^6}$ which is negative provided $\kappa_{y_2} \neq 0$. Hence if $\kappa_{y_2} \neq 0$ any interior point is a saddle. If $\kappa_{y_2} = 0$ then $\frac{\partial}{\partial x_1} = -A \neq 0$, hence there are no interior critical points to begin with.

Case 3) Fixed y_1, x_2 to κ_{y_1} and κ_{x_2} respectively. In this case the 2D Hessian determinant is $\frac{-1}{x_2^2}$ which is always strictly negative, hence any potential critical point would necessarily be a saddle point and thus not a local extrema.

Case 4) Fixed x_1, y_2 to κ_{x_1} and κ_{y_2} respectively. In this case the 2D Hessian determinant is also $\frac{-1}{x_2^2}$ which is always strictly negative, hence any potential critical point would necessarily be a saddle point and thus not a local extrema.

Case 5) Fixed x_1, x_2 to κ_{x_1} and κ_{x_2} respectively. In this case the function $\frac{(x_2 \cdot y_1) - (x_1 \cdot y_2)}{x_2^2} - (Ax_1 + By_1 + Cx_2 + Dy_2 + E)$ becomes linear in both dimensions, and the optimal values will occur at the corner points and hence there are no interior critical points. Case 6) Fixed x_1, y_1 to κ_{x_1} and κ_{y_1} respectively. In this case the Hessian determinant is $\frac{-4\kappa_{x_1}^2}{x_2^6}$ which is negative provided $\kappa_{x_1} \neq 0$ hence any interior critical point is necessarily a saddle point. If $\kappa_{x_1} = 0$, then $\frac{\partial}{\partial y_2} = -D \neq 0$, thus there is no critical point to begin with. \square

A.4.3 1D Subproblems.

PROOF. Case 1) Fix every variable to its lower or upper bounds *except* x_1 . In this case the function becomes linear and thus the extrema will occur at either $x_1 = l_{x_1}$ or $x_1 = u_{x_1}$

Case 2) Fix every variable to its lower or upper bounds *except* y_1 . In this case the function still is linear. and thus the extrema will occur at either $y_1 = l_{y_1}$ or $y_1 = u_{y_1}$

Case 3) Fixed every variable to its lower or upper bounds *except* x_2 . In this case the function is *not* linear hence we have to solve for critical points, however thankfully this is now only a univariate problem. We have to solve for $x_2 \in [l_{x_2}, u_{x_2}]$ such that $\frac{\partial}{\partial x_2} = \frac{2\kappa_{x_1}\kappa_{y_2} - \kappa_{y_1}x_2}{x_2^3} - C = 0$. Hence we must solve the 3rd degree polynomial $Cx_2^3 + \kappa_{y_1}x_2 - 2\kappa_{x_1}\kappa_{y_2} = 0$. However because $\kappa_{x_1}, \kappa_{y_1}, \kappa_{y_2}$ each could be the respective lower *or* upper bounds, this means we must actually solve 8 versions of this 3rd degree (univariate) polynomial. However this can still easily be done analytically, and thus we would check if each of the 8 equations has a root in $[l_{x_2}, u_{x_2}]$

Case 4) Fix every variable to its lower or upper bounds *except* y_2 . In this case the function still is linear and thus the extrema will occur at either $y_2 = l_{y_2}$ or $y_2 = u_{y_2}$ \square

A.4.4 0D Subproblems. We just enumerate over all 2^4 corners: $(x_1, y_1, x_2, y_2) \in \{l_{x_1}, u_{x_1}\} \times \{l_{y_1}, u_{y_1}\} \times \{l_{x_2}, u_{x_2}\} \times \{l_{y_2}, u_{y_2}\}$

A.5 Full Quotient Rule Proof for Intervals

We now detail the rest of the cases for the quotient rule for the Interval case

A.5.1 3D Subproblems.

PROOF. Case 1) Fixed y_2 to either l_{y_2} or u_{y_2} - we denote the fixed constant value of y_2 as κ_{y_2} , hence $\kappa_{y_2} \in \{l_{y_2}, u_{y_2}\}$. In this case the first derivatives are:

$$\begin{aligned} \frac{\partial}{\partial x_1} &= \frac{\kappa_{y_2}}{x_2^2} \\ \frac{\partial}{\partial y_1} &= \frac{1}{x_2} \\ \frac{\partial}{\partial x_2} &= \frac{2x_1\kappa_{y_2} - y_1x_2}{x_2^3} \end{aligned}$$

Since the range $[l_{x_2}, u_{x_2}]$ excludes zero, this ensures that $\frac{\partial}{\partial y_1} = \frac{1}{x_2}$ is never zero

Case 2) Fixed x_2 to either l_{x_2} or u_{x_2} - we denote the fixed constant value of x_2 as κ_{x_2} . In this case the first derivatives are:

$$\begin{aligned}\frac{\partial}{\partial x_1} &= \frac{y_2}{\kappa_{x_2}^2} \\ \frac{\partial}{\partial y_1} &= \frac{1}{\kappa_{x_2}} \\ \frac{\partial}{\partial y_2} &= \frac{x_1}{\kappa_{x_2}^2}\end{aligned}$$

Since the range $[l_{x_2}, u_{x_2}]$ excludes zero, this ensures $\kappa_{x_2} \neq 0$, hence $\frac{\partial}{\partial y_1} = \frac{1}{\kappa_{x_2}}$ is never zero

Case 3) Fixed y_1 to either l_{y_1} or u_{y_1} - we denote the fixed constant value of y_1 as κ_{y_1} , hence $\kappa_{y_1} \in \{l_{y_1}, u_{y_1}\}$. In this case the first derivatives are:

$$\begin{aligned}\frac{\partial}{\partial x_1} &= \frac{-y_2}{x_2^2} \\ \frac{\partial}{\partial x_2} &= \frac{2x_1y_2 - \kappa_{y_1}x_2}{x_2^3} \\ \frac{\partial}{\partial y_2} &= \frac{-x_1}{x_2^2}\end{aligned}$$

Case 3.1) $\kappa_{y_1} \neq 0$. Since $x_2 \neq 0$, the only way for $\frac{\partial}{\partial x_1} = \frac{\partial}{\partial y_2} = \frac{\partial}{\partial x_2} = 0$ is if $x_1 = y_2 = 0$ and $\kappa_{y_1} = 0$, hence if $\kappa \neq 0$, then it is not possible for $\frac{\partial}{\partial x_2}$ to be zero.

Case 3.2) $\kappa_{y_1} = 0$. In this case if $[l_{x_1}, u_{x_1}]$ and $[l_{y_2}, u_{y_2}]$ both include 0, then we could have a critical point that the Hessian test cannot immediately rule out. However the value of the function at this critical point is always 0, hence it suffices to add a single additional point (0) to the finite list of points to check

Case 4) Fixed x_1 to either l_{x_1} or u_{x_1} - we denote the fixed constant value of x_1 as κ_{x_1} . In this case the first derivatives are:

$$\begin{aligned}\frac{\partial}{\partial y_1} &= \frac{1}{x_2} \\ \frac{\partial}{\partial x_2} &= \frac{2\kappa_{x_1}y_2 - y_1x_2}{x_2^3} \\ \frac{\partial}{\partial y_2} &= \frac{\kappa_{x_1}}{x_2^2}\end{aligned}$$

Since the range $[l_{x_2}, u_{x_2}]$ excludes zero, this ensures that $\frac{\partial}{\partial y_1} = \frac{1}{x_2}$ is never zero. \square

A.5.2 2D Subproblems.

PROOF. Case 1) Fixed x_2, y_2 to κ_{x_2} and κ_{y_2} respectively. In this case the function $\frac{(x_2 \cdot y_1) - (x_1 \cdot y_2)}{x_2^2}$ becomes linear in both dimensions, and the optimal values (both min *and* max) will occur at the corner points and hence there are no interior critical points.

Case 2) Fixed y_1, y_2 to κ_{y_1} and κ_{y_2} respectively. The 2D Hessian determinant in this 2D subproblem is $\frac{-4\kappa_{y_2}^2}{x_2^6}$ which is negative provided $\kappa_{y_2} \neq 0$. Hence if $\kappa_{y_2} \neq 0$ any interior point is a saddle. If $\kappa_{y_2} = 0$ then the function $\frac{(x_2 \cdot y_1) - (x_1 \cdot y_2)}{x_2^2}$ becomes $\frac{\kappa_{y_1}}{x_2}$, hence $\frac{\partial}{\partial x_2} = \frac{-\kappa_{y_1}}{x_2^2}$ which is non-zero provided $\kappa_{y_1} \neq 0$. If κ_{y_1} and $\kappa_{y_2} = 0$, then the function is everywhere 0, which will be caught when we check corner points.

Case 3) Fixed y_1, x_2 to κ_{y_1} and κ_{x_2} respectively. In this case the 2D Hessian determinant is $\frac{-1}{x_2^4}$ which is always strictly negative, hence any potential critical point would necessarily be a saddle point and thus not a local extrema.

Case 4) Fixed x_1, y_2 to κ_{x_1} and κ_{y_2} respectively. In this case the 2D Hessian determinant is also $\frac{-1}{x_2^4}$ which is always strictly negative, hence any potential critical point would necessarily be a saddle point and thus not a local extrema.

Case 5) Fixed x_1, x_2 to κ_{x_1} and κ_{x_2} respectively. In this case the function $\frac{(x_2 \cdot y_1) - (x_1 \cdot y_2)}{x_2^2}$ becomes linear in both dimensions, and the optimal values will occur at the corner points and hence there are no interior critical points.

Case 6) Fixed x_1, y_1 to κ_{x_1} and κ_{y_1} respectively. In this case the Hessian determinant is $\frac{-4\kappa_{x_1}^2}{x_2^6}$ which is negative provided $\kappa_{x_1} \neq 0$ hence any interior critical point is necessarily a saddle point. If $\kappa_{x_1} = 0$, then the function $\frac{(x_2 \cdot y_1) - (x_1 \cdot y_2)}{x_2^2}$ becomes $\frac{\kappa_{y_1}}{x_2}$, hence $\frac{\partial}{\partial x_2} = \frac{-\kappa_{y_1}}{x_2^2}$ which is non-zero provided $\kappa_{y_1} \neq 0$. If κ_{y_1} and $\kappa_{x_1} = 0$, then the function is everywhere 0, which will be caught when we check corner points. \square

A.5.3 1D Subproblems.

PROOF. Case 1) Fix every variable to its lower or upper bounds *except* x_1 . In this case the function becomes linear and thus the extrema will occur at either $x_1 = l_{x_1}$ or $x_1 = u_{x_1}$

Case 2) Fix every variable to its lower or upper bounds *except* y_1 . In this case the function still is linear. and thus the extrema will occur at either $y_1 = l_{y_1}$ or $y_1 = u_{y_1}$

Case 3) Fixed every variable to its lower or upper bounds *except* x_2 . In this case the function is *not* linear hence we have to solve for critical points, however thankfully this is now only a univariate problem. We have to solve for $x_2 \in [l_{x_2}, u_{x_2}]$ such that $\frac{\partial}{\partial x_2} = \frac{2\kappa_{x_1}\kappa_{y_2} - \kappa_{y_1}x_2}{x_2^3} = 0$. Hence we must solve $2\kappa_{x_1}\kappa_{y_2} - \kappa_{y_1}x_2 = 0$. Hence for each possible root $x_2 = \frac{2\kappa_{x_1}\kappa_{y_2}}{\kappa_{y_1}}$, we must check if $\frac{2\kappa_{x_1}\kappa_{y_2}}{\kappa_{y_1}} \in [l_{x_2}, u_{x_2}]$, and if so we will need to evaluate the function $\frac{(x_2 \cdot y_1) - (x_1 \cdot y_2)}{x_2^2}$ at said critical point. We keep in mind that there are really 8 versions of this equation that we must resolve.

Case 4) Fix every variable to its lower or upper bounds *except* y_2 . In this case the function still is linear and thus the extrema will occur at either $y_2 = l_{y_2}$ or $y_2 = u_{y_2}$ \square

A.5.4 0D Subproblems. We just enumerate over all 2^4 corners: $(x_1, y_1, x_2, y_2) \in \{l_{x_1}, u_{x_1}\} \times \{l_{y_1}, u_{y_1}\} \times \{l_{x_2}, u_{x_2}\} \times \{l_{y_2}, u_{y_2}\}$

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