

Fundamentals of Unconstrained Optimization

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Abstract

As formal methods gain traction in machine learning and numerical analysis, the community needs computer-checked proofs of core optimization results. Existing Isabelle libraries still lack a foundational framework for unconstrained optimization. We close this gap with a comprehensive Isabelle/HOL development that formalizes:

- (1) minimizers, strict and isolated local minimizers;
- (2) first- and second-order optimality conditions for scalar functions $f : \mathbb{R} \rightarrow \mathbb{R}$;
- (3) first-order optimality conditions for vector functions $g : \mathbb{R}^n \rightarrow \mathbb{R}$; and
- (4) a worked example showing that the continuous function

$$h(x) = \begin{cases} x^4(\cos(1/x) + 2), & x \neq 0, \\ 0, & x = 0 \end{cases}$$

has a *strict* but *non-isolated* local minimizer at $x = 0$.

The new session `Unconstrained_Optimization` provides sound, reusable foundations for future proof-checking tools and mechanized research in optimization, analysis, and algorithmic correctness.

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1 Auxiliary Facts

theory *Auxiliary-Facts*

imports

Sigmoid-Universal-Approximation.Limits-Higher-Order-Derivatives

begin

1.1 Differentiation Lemmas

lemma *has-derivative-imp*:

fixes $f :: real \Rightarrow real$

assumes $(f \text{ has-derivative } f') (at\ x)$

shows $f \text{ differentiable } (at\ x) \wedge deriv\ f\ x = f'\ 1$

<proof>

lemma *DERIV-inverse-func*:

assumes $x \neq 0$

shows $DERIV (\lambda w. 1 / w)\ x :> -1 / x^2$

<proof>

lemma *power-rule*:

fixes $z :: real$ and $n :: nat$

shows $deriv (\lambda x. x^n)\ z = (if\ n = 0\ then\ 0\ else\ real\ n * z^{n-1})$

<proof>

1.1.1 Transfer Lemmas

lemma *has-derivative-transfer-on-ball*:

fixes $f\ g :: real \Rightarrow real$

assumes $eps-gt0: 0 < \varepsilon$

assumes $eq-on-ball: \forall y. y \in ball\ x\ \varepsilon \longrightarrow f\ y = g\ y$

assumes $f\text{-has-deriv}: (f \text{ has-derivative } D) (at\ x)$

shows $(g \text{ has-derivative } D) (at\ x)$

<proof>

corollary *field-differentiable-transfer-on-ball:*

fixes $f\ g :: \text{real} \Rightarrow \text{real}$

assumes $0 < \varepsilon$

assumes *eq-on-ball*: $\forall y. y \in \text{ball } x\ \varepsilon \longrightarrow f\ y = g\ y$

assumes *f-diff*: f *field-differentiable at* x

shows g *field-differentiable at* x

<proof>

1.2 Trigonometric Contraction

lemma *cos-contractive:*

fixes $x\ y :: \text{real}$

shows $|\cos x - \cos y| \leq |x - y|$

<proof>

lemma *sin-contractive:*

fixes $x\ y :: \text{real}$

shows $|\sin x - \sin y| \leq |x - y|$

<proof>

1.3 Algebraic Factorizations

lemma *biquadrate-diff-biquadrate-factored:*

fixes $x\ y :: \text{real}$

shows $y^4 - x^4 = (y - x) * (y^3 + y^2 * x + y * x^2 + x^3)$

<proof>

1.4 Specific Trigonometric Values

lemma *sin-5pi-div-4*: $\sin (5 * \text{pi} / 4) = - (\text{sqrt } 2 / 2)$

<proof>

lemma *cos-5pi-div-4*: $\cos (5 * \text{pi} / 4) = - (\text{sqrt } 2 / 2)$

<proof>

1.5 Local Sign Preservation of Continuous Functions

1.5.1 Local Positivity

lemma *cont-at-pos-imp-loc-pos:*

fixes $g :: \text{real} \Rightarrow \text{real}$ **and** $x :: \text{real}$

assumes *continuous (at x) g* **and** $g\ x > 0$

shows $\exists \delta > 0. \forall y. |y - x| < \delta \longrightarrow g\ y > 0$

<proof>

lemma *cont-at-pos-imp-loc-pos'*:

fixes $g :: \text{real} \Rightarrow \text{real}$ **and** $x :: \text{real}$

assumes *continuous (at x) g* **and** $g\ x > 0$

shows $\exists \Delta > 0. \forall \delta. 0 < \delta \wedge \delta \leq \Delta \longrightarrow (\forall y. |y - x| < \delta \longrightarrow g y > 0)$
 <proof>

1.5.2 Local Negativity

lemma *cont-at-neg-imp-loc-neg*:
fixes $g :: real \Rightarrow real$ **and** $x :: real$
assumes *continuous (at x) g* **and** $g x < 0$
shows $\exists \delta > 0. \forall y. |y - x| < \delta \longrightarrow g y < 0$
 <proof>

lemma *cont-at-neg-imp-loc-neg'*:
fixes $g :: real \Rightarrow real$ **and** $x :: real$
assumes *continuous (at x) g* **and** $g x < 0$
shows $\exists \Delta > 0. \forall \delta. 0 < \delta \wedge \delta \leq \Delta \longrightarrow (\forall y. |y - x| < \delta \longrightarrow g y < 0)$
 <proof>

end

2 Minimizers in Topological and Metric Spaces

theory *Minimizers-Definition*
imports *Auxiliary-Facts*
begin

2.1 Abstract Topological Definitions

definition *global-minimizer* :: $('a::topological-space \Rightarrow real) \Rightarrow 'a \Rightarrow bool$ **where**
global-minimizer $f x\text{-star} \longleftrightarrow (\forall x. f x\text{-star} \leq f x)$

definition *local-minimizer-on* :: $('a::topological-space \Rightarrow real) \Rightarrow 'a \Rightarrow 'a\ set \Rightarrow bool$ **where**
local-minimizer-on $f x\text{-star} U \longleftrightarrow (open\ U \wedge x\text{-star} \in U \wedge (\forall x \in U. f x\text{-star} \leq f x))$

definition *local-minimizer* :: $('a::topological-space \Rightarrow real) \Rightarrow 'a \Rightarrow bool$ **where**
local-minimizer $f x\text{-star} \longleftrightarrow (\exists U. open\ U \wedge x\text{-star} \in U \wedge (\forall x \in U. f x\text{-star} \leq f x))$

definition *isolated-local-minimizer-on* :: $('a::topological-space \Rightarrow real) \Rightarrow 'a \Rightarrow 'a\ set \Rightarrow bool$ **where**
isolated-local-minimizer-on $f x\text{-star} U \longleftrightarrow$
 $(local\text{-minimizer}\text{-on}\ f\ x\text{-star}\ U \wedge (\{x \in U. local\text{-minimizer}\ f\ x\} = \{x\text{-star}\}))$

definition *isolated-local-minimizer* :: $('a::topological-space \Rightarrow real) \Rightarrow 'a \Rightarrow bool$ **where**
isolated-local-minimizer $f x\text{-star} \longleftrightarrow$
 $(\exists U. local\text{-minimizer}\text{-on}\ f\ x\text{-star}\ U \wedge (\{x \in U. local\text{-minimizer}\ f\ x\} = \{x\text{-star}\}))$

definition *strict-local-minimizer-on* :: ('a::topological-space \Rightarrow real) \Rightarrow 'a \Rightarrow 'a set \Rightarrow bool **where**

strict-local-minimizer-on f x-star U \longleftrightarrow
 (open U \wedge x-star \in U \wedge ($\forall x \in U - \{x\text{-star}\}, f\ x\text{-star} < f\ x$))

definition *strict-local-minimizer* :: ('a::topological-space \Rightarrow real) \Rightarrow 'a \Rightarrow bool **where**

strict-local-minimizer f x-star \longleftrightarrow ($\exists U. \text{strict-local-minimizer-on } f\ x\text{-star } U$)

2.2 Metric Space Reformulations

lemma *local-minimizer-on-def2*:

fixes f :: 'a::metric-space \Rightarrow real
assumes *local-minimizer* f x-star
shows $\exists N > 0. \forall x \in \text{ball } x\text{-star } N. f\ x\text{-star} \leq f\ x$
 <proof>

lemma *local-minimizer-def2*:

fixes f :: 'a::metric-space \Rightarrow real
assumes *local-minimizer* f x-star
shows $\exists N > 0. \forall x. \text{dist } x\ x\text{-star} < N \longrightarrow f\ x\text{-star} \leq f\ x$
 <proof>

lemma *isolated-local-minimizer-on-def2*:

fixes f :: 'a::metric-space \Rightarrow real
assumes *isolated-local-minimizer-on* f x-star U
shows $\exists N > 0. \forall x \in \text{ball } x\text{-star } N. (\text{local-minimizer } f\ x \longrightarrow x = x\text{-star})$
 <proof>

lemma *isolated-local-minimizer-def2*:

fixes f :: 'a::metric-space \Rightarrow real
assumes *isolated-local-minimizer* f x-star
shows $\exists N > 0. \forall x \in \text{ball } x\text{-star } N. (\text{local-minimizer } f\ x \longrightarrow x = x\text{-star})$
 <proof>

lemma *strict-local-minimizer-on-def2*:

fixes f :: 'a::metric-space \Rightarrow real
assumes *strict-local-minimizer-on* f x-star U
shows $\exists N > 0. \forall x \in \text{ball } x\text{-star } N - \{x\text{-star}\}. f\ x\text{-star} < f\ x$
 <proof>

lemma *strict-local-minimizer-def2*:

fixes f :: 'a::metric-space \Rightarrow real
assumes *strict-local-minimizer* f x-star
shows $\exists N > 0. \forall x \in \text{ball } x\text{-star } N - \{x\text{-star}\}. f\ x\text{-star} < f\ x$
 <proof>

lemma *local-minimizer-neighborhood*:

fixes f :: real \Rightarrow real

assumes *loc-min: local-minimizer f x-min*
shows $\exists \delta > 0. \forall h. |h| < \delta \longrightarrow f (x\text{-min} + h) \geq f x\text{-min}$
<proof>

lemma *local-minimizer-from-neighborhood:*
fixes $f :: \text{real} \Rightarrow \text{real}$ **and** $x\text{-min} :: \text{real}$
assumes $\exists \delta > 0. \forall x. |x - x\text{-min}| < \delta \longrightarrow f x\text{-min} \leq f x$
shows *local-minimizer f x-min*
<proof>

end

3 Minimizer Implications

theory *First-Order-Conditions*
imports *Minimizers-Definition*
begin

notation *norm* ($\|-\|$)

3.1 Implications for a Given Minimizer Type

lemma *strict-local-minimizer-imp-local-minimizer:*
assumes *strict-local-minimizer f x-star*
shows *local-minimizer f x-star*
<proof>

lemma *isolated-local-minimizer-imp-strict:*
assumes *isolated-local-minimizer f x-star*
shows *strict-local-minimizer f x-star*
<proof>

3.2 Characterization of Non-Isolated Minimizers

lemma *not-isolated-minimizer-def:*
assumes *local-minimizer f x-star*
shows $(\exists x\text{-seq} :: \text{nat} \Rightarrow \text{real}. (\forall n. \text{local-minimizer } f (x\text{-seq } n) \wedge x\text{-seq } n \neq x\text{-star})$
 $\wedge ((x\text{-seq} \longrightarrow x\text{-star}) \text{ at-top})) = (\neg \text{isolated-local-minimizer } f x\text{-star})$
<proof>

3.3 First-Order Condition

theorem *Fermat's-theorem-on-stationary-points:*
fixes $f :: \text{real} \Rightarrow \text{real}$
assumes $(f \text{ has-derivative } f')$ *(at x-min)*
assumes *local-minimizer f x-min*
shows $(\text{deriv } f) x\text{-min} = 0$
<proof>

definition *stand-basis-vector* :: 'n::finite \Rightarrow realⁿ — the i-th standard basis vector

where *stand-basis-vector* i = (χ j. if j = i then 1 else 0)

lemma *stand-basis-vector-index[simp]*: (*stand-basis-vector* i) \$ j = (if j = i then (1::real) else 0)
 ⟨proof⟩

lemma *stand-basis-vector-nonzero[simp]*: *stand-basis-vector* i \neq 0
 ⟨proof⟩

lemma *norm-stand-basis-vector[simp]*: norm (*stand-basis-vector* i) = 1
 ⟨proof⟩

lemma *inner-stand-basis-vector[simp]*: inner (*stand-basis-vector* i) (*stand-basis-vector* j) = (if i = j then 1 else 0)
 ⟨proof⟩

lemma *Basis-characterisation*:
stand-basis-vector i \in (*Basis* :: (realⁿ) set) **and**
 $\forall b \in$ (*Basis*::(realⁿ)set). $\exists i. b =$ *stand-basis-vector* i
 ⟨proof⟩

lemma *stand-basis-expansion*:
fixes x :: realⁿ
shows x = (\sum j \in UNIV. (x \$ j) *_R *stand-basis-vector* j)
 ⟨proof⟩

lemma *has-derivative-affine*:
fixes a v :: 'a::real-normed-vector
shows ((λ t. a + t *_R v) has-derivative (λ h. h *_R v)) (at x)
 ⟨proof⟩

theorem *Fermat's-theorem-on-stationary-points-mult*:
fixes f :: realⁿ \Rightarrow real
assumes der-f: (f has-derivative f') (at x-min)
assumes min-f: local-minimizer f x-min
shows GDERIV f x-min :> 0
 ⟨proof⟩

end

4 Second-Order Conditions

theory *Second-Derivative-Test*
imports *First-Order-Conditions*
begin

4.1 Necessary Condition

lemma *snd-derivative-nonneg-at-local-min-necessary*:
fixes $f :: \text{real} \Rightarrow \text{real}$
assumes *C2-cont-diff-at-xmin*: $C\text{-k-on } 2 f (U :: \text{real set})$
assumes *min-in-U*: $(x\text{-min} :: \text{real}) \in U$
assumes *loc-min*: $\text{local-minimizer } f x\text{-min}$
shows $\text{deriv } (\text{deriv } f) x\text{-min} \geq 0$
<proof>

4.2 Sufficient Condition

lemma *second-derivative-test*:
fixes $f :: \text{real} \Rightarrow \text{real}$ **and** $a :: \text{real}$ **and** $b :: \text{real}$ **and** $x\text{-min} :: \text{real}$
assumes *valid-interval*: $a < b$
assumes *twice-continuously-differentiable*: $C\text{-k-on } 2 f \{a <..< b\}$
assumes *min-exists*: $x\text{-min} \in \{a <..< b\}$
assumes *fst-deriv-req*: $(\text{deriv } f) x\text{-min} = 0$
assumes *snd-deriv-req*: $\text{deriv } (\text{deriv } f) x\text{-min} > 0$
shows *loc-min*: $\text{local-minimizer } f x\text{-min}$
<proof>

end

5 Pathological Example: Non-Isolated Strict Local Minima

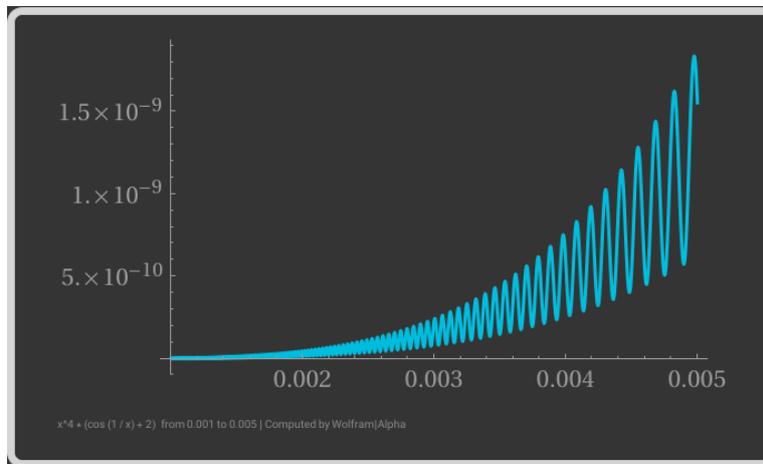
theory *Cont-Nonisolated-Strict-Local-Minimizer-Exists*
imports *Second-Derivative-Test HOL-Library.Quadratic-Discriminant*
begin

Idea of the example. We construct a continuous function

$$f(x) = \begin{cases} x^4(\cos(1/x) + 2), & x \neq 0, \\ 0, & x = 0 \end{cases}$$

whose oscillations *speed up* as $x \rightarrow 0$ because of the $\cos(1/x)$ term. Multiplying by x^4 makes the function and its first derivative vanish at the origin, ensuring that $x = 0$ is a strict local minimizer, while the shifted cosine creates infinitely many additional strict local minimizers that accumulate at 0. Hence the minimizer at 0 is *strict* but *not isolated*.

theorem *Exists-Continuous-Func-with-non-isolated-strict-local-minimizer*:
 $\exists f :: \text{real} \Rightarrow \text{real}.$ *continuous-on* $\mathbb{R} f \wedge$
 $(\exists x\text{-star}.$ *strict-local-minimizer } f x\text{-star} \wedge \neg \text{isolated-local-minimizer } f x\text{-star})
*<proof>**



```

end
theory Unconstrained-Optimization
  imports Auxiliary-Facts
         Minimizers-Definition
         First-Order-Conditions
         Second-Derivative-Test
         Cont-Nonisolated-Strict-Local-Minimizer-Exists
begin
end

```

References

- [1] T. Nipkow, M. Wenzel, and L. C. Paulson. *Isabelle/HOL: A Proof Assistant for Higher-Order Logic*, volume 2283 of *Lecture Notes in Computer Science*. Springer, Berlin, Heidelberg, 2002.
- [2] J. Nocedal and S. J. Wright. *Numerical Optimization*. Springer Series in Operations Research and Financial Engineering. Springer, New York, second edition, 2006.