

Simple Optimization Problems

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Computational Mathematics for Learning and Data Analysis
Master in Computer Science – University of Pisa

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Outline

Optimization Problems

Optimization is difficult

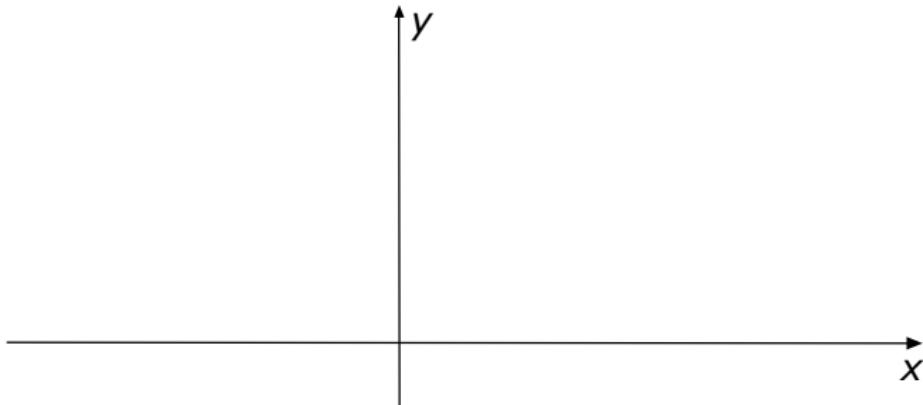
Simple Functions, Univariate case

Simple Functions, Multivariate case

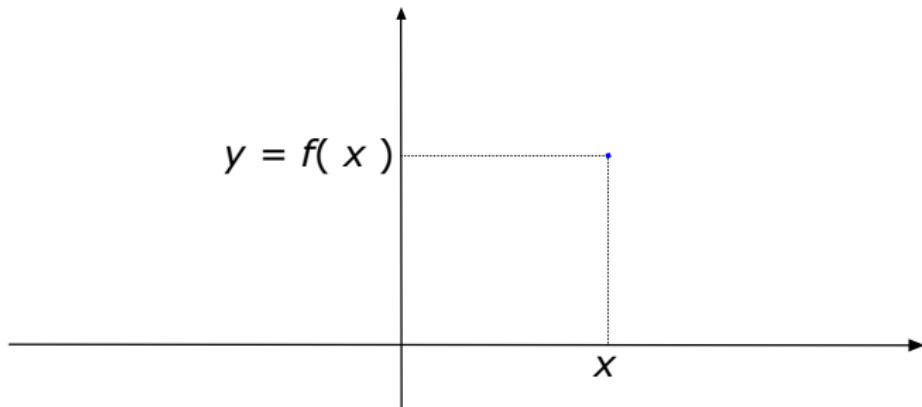
Multivariate Quadratic case: Gradient Method

Wrap up & References

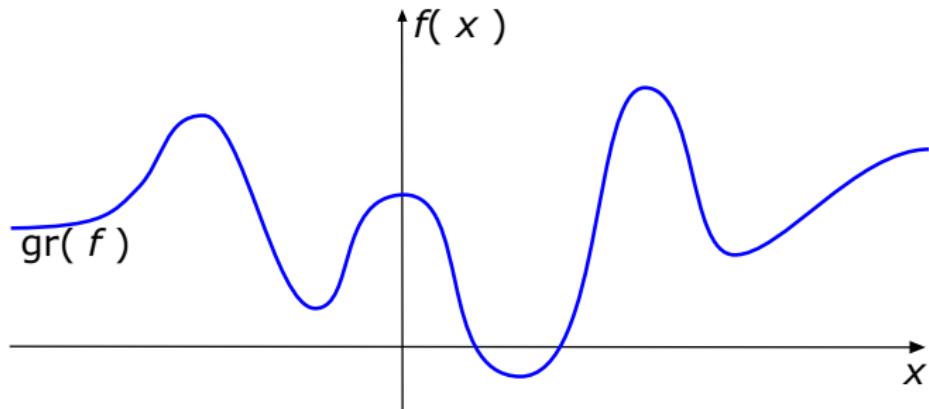
Solutions



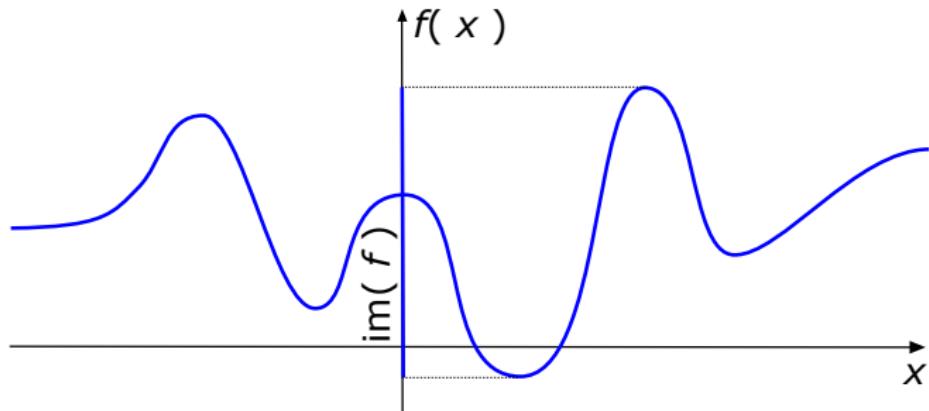
- ▶ Let's start simple: x input space, y output space, both just \mathbb{R}



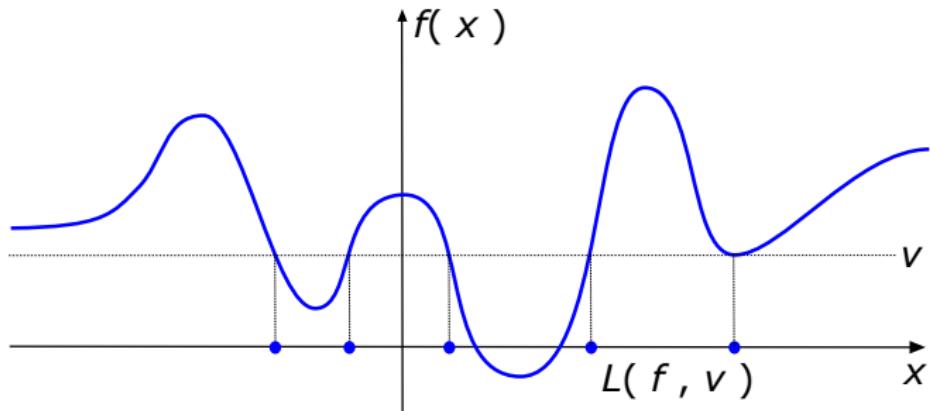
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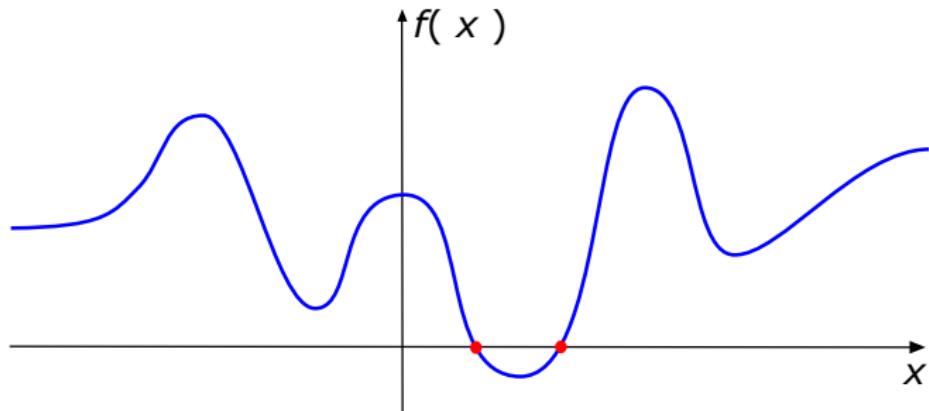
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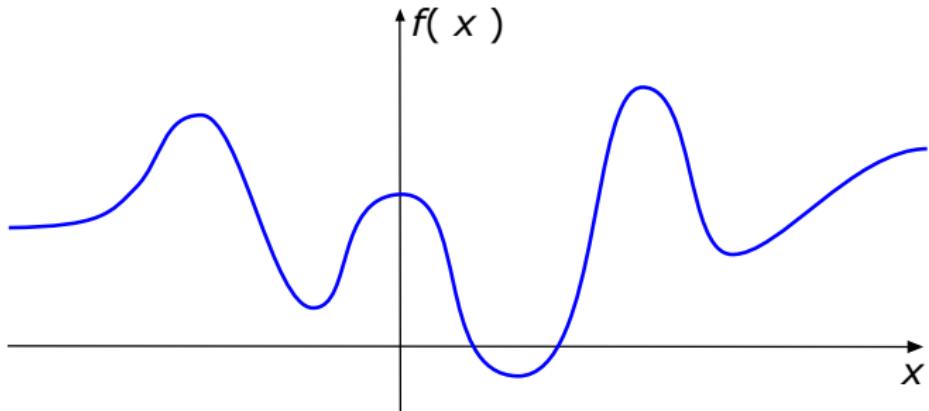
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(roots of $f = L(f, 0)$ = level set at value 0)

(Univariate) Unconstrained optimization problem

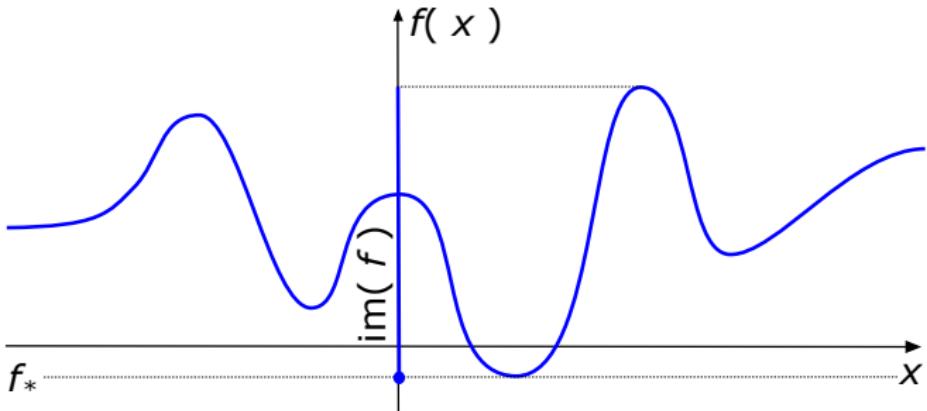
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- ▶ f objective (function) of (univariate, unconstrained) optimization problem
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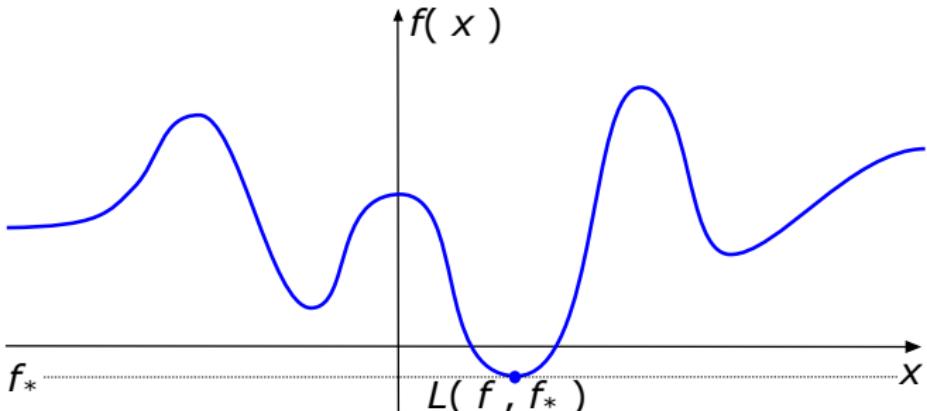
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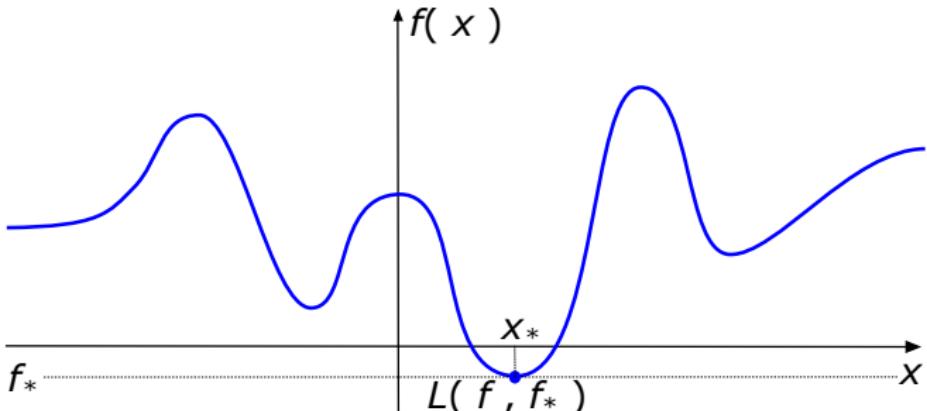
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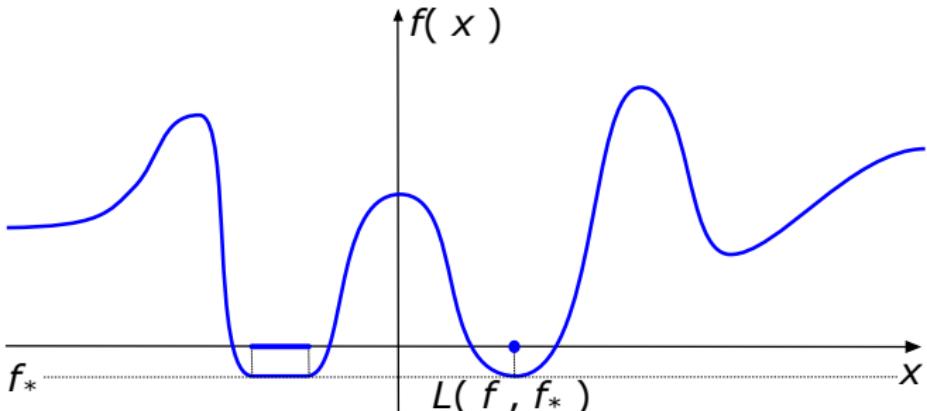
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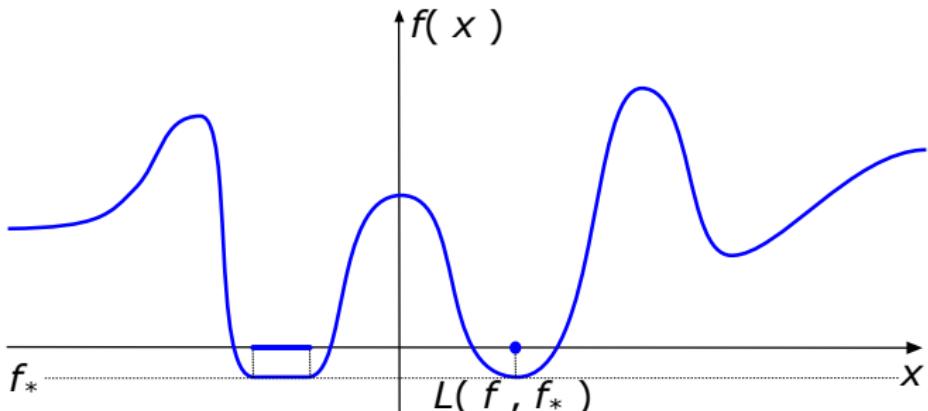
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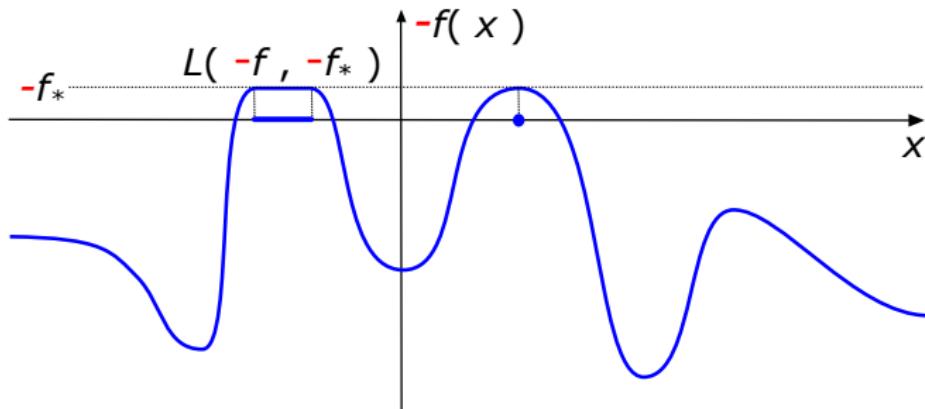
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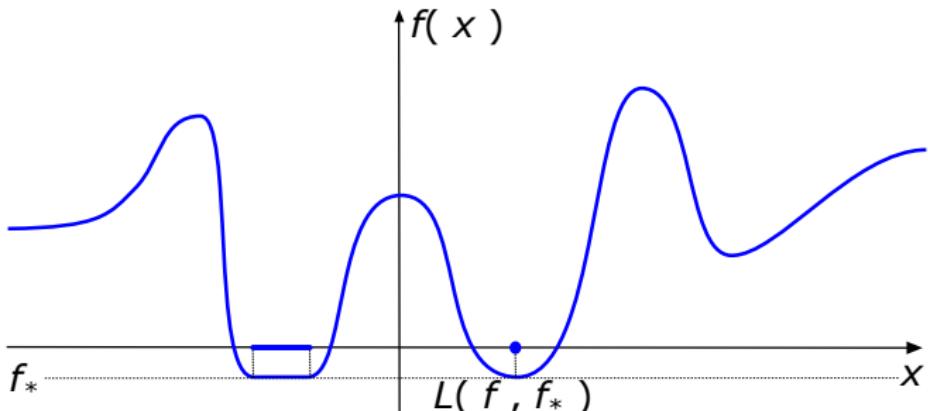
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- ▶ x_* may not be unique: $\exists x' \neq x_* \in L(f, f_*) = X_*$ set of optimal solutions, but we don't care (mostly): all optimal solutions equivalent "in the eyes of f "



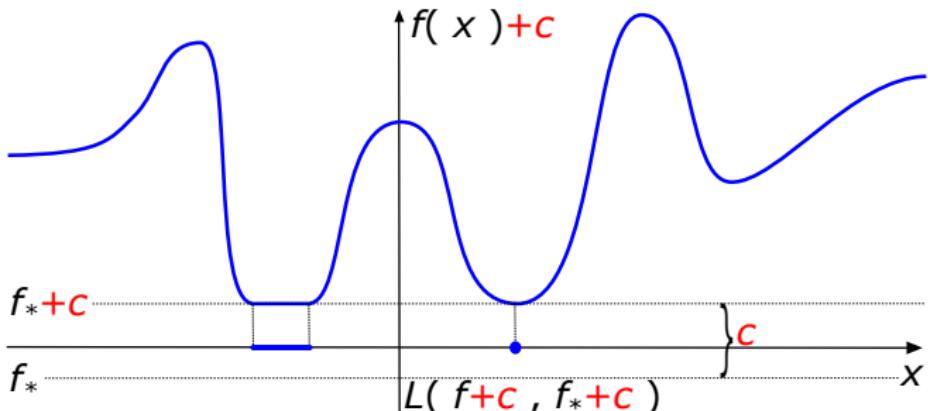
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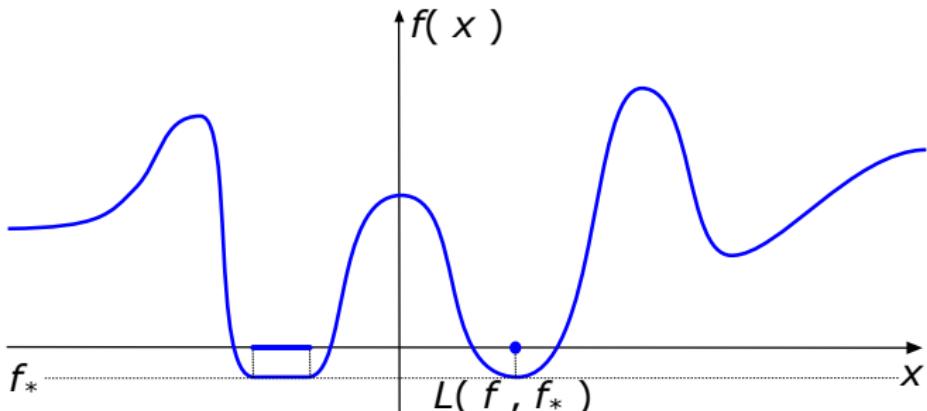
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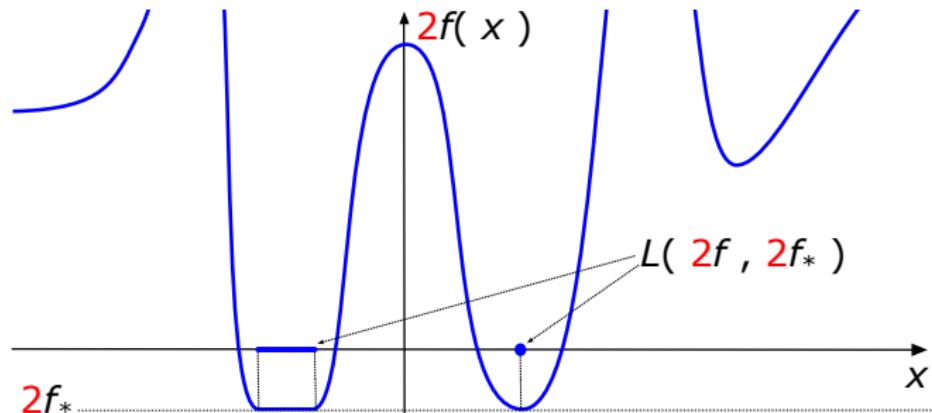
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An aside, once and for all: simple reformulations

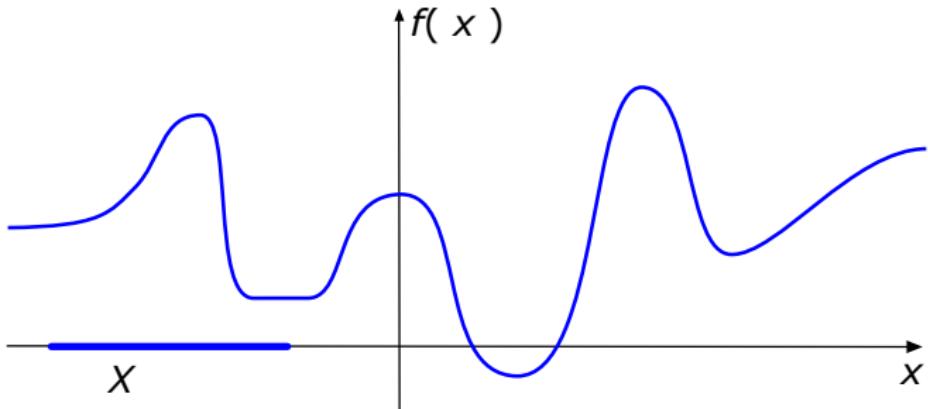
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(Univariate) Constrained optimization problem

4

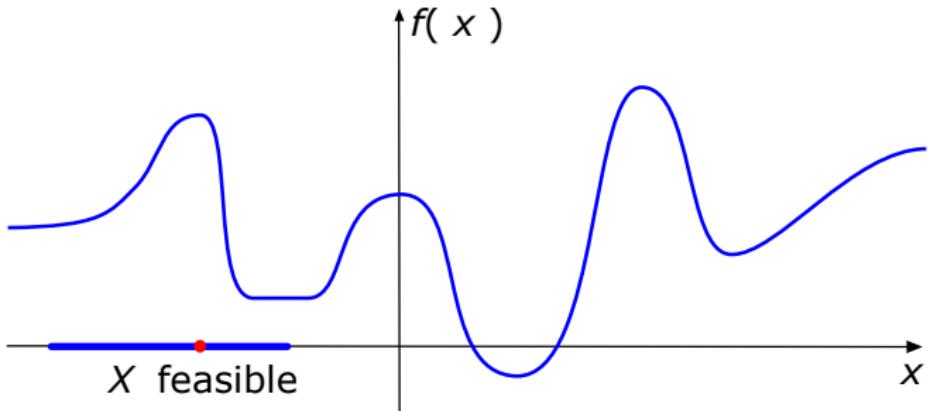


► More general: **feasible region** **any** set X ($\subseteq \mathbb{R}$), objective $f : X \rightarrow \mathbb{R}$

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(Univariate) Constrained optimization problem

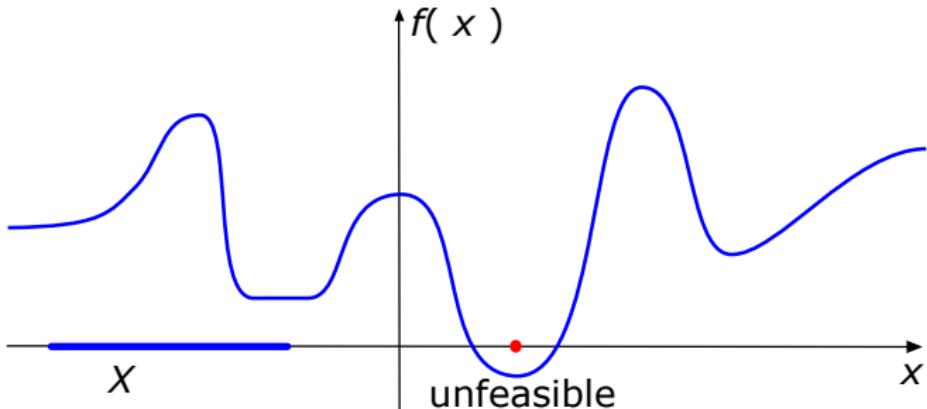
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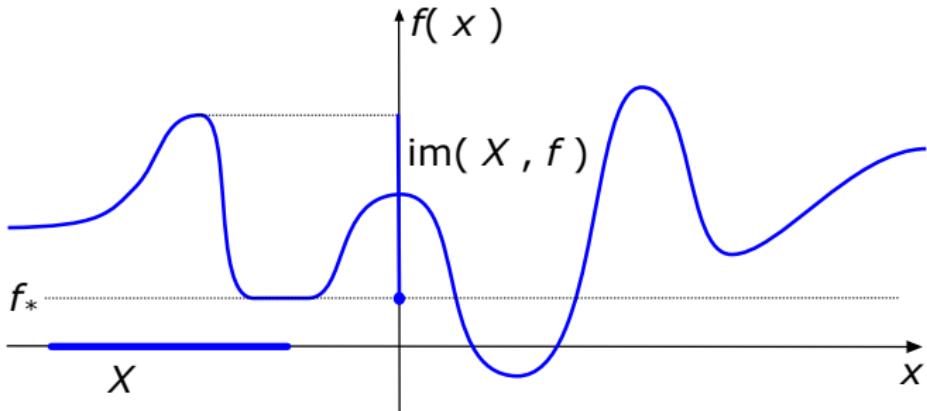
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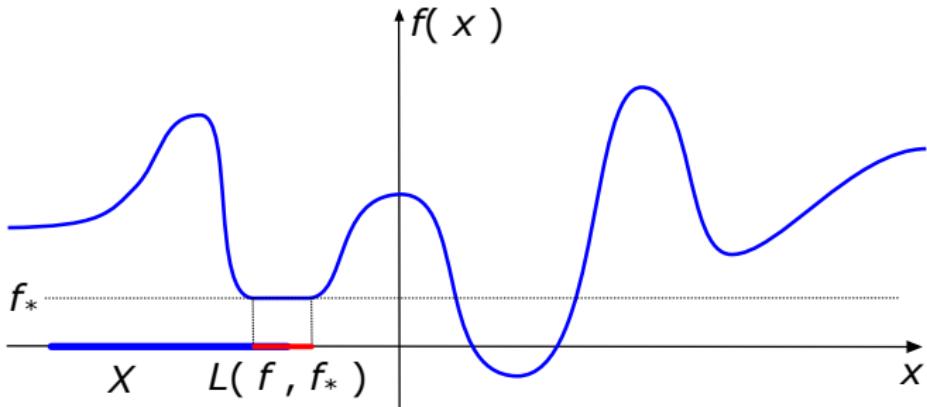
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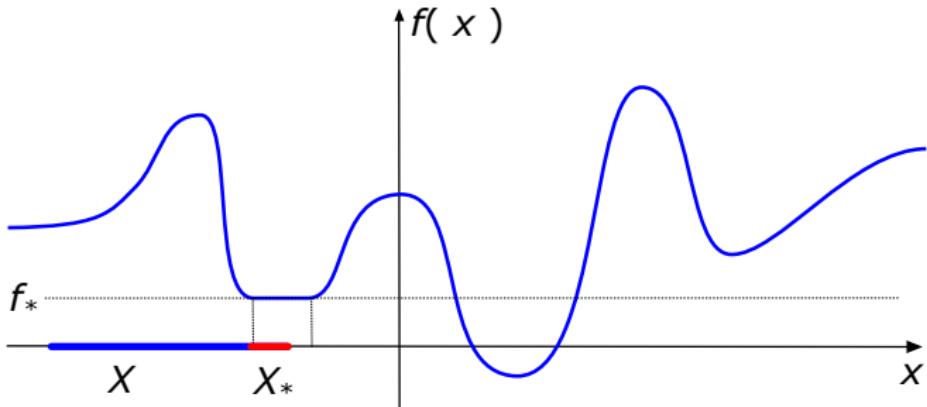
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- ▶ $X_* = L(f, f_*)$

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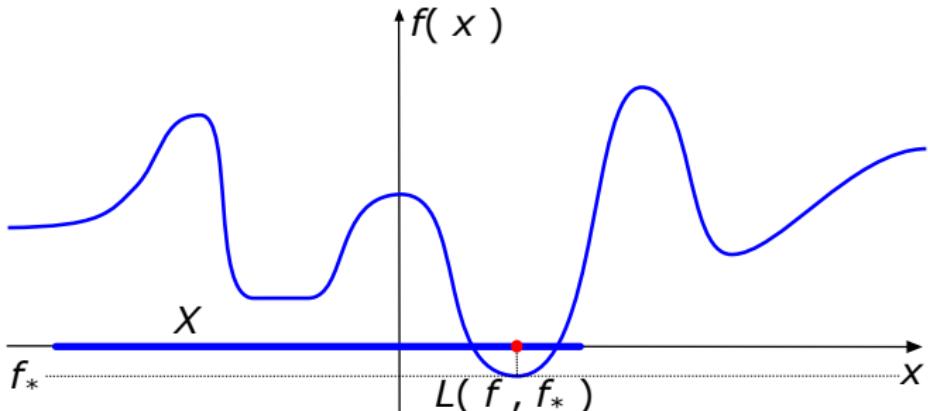
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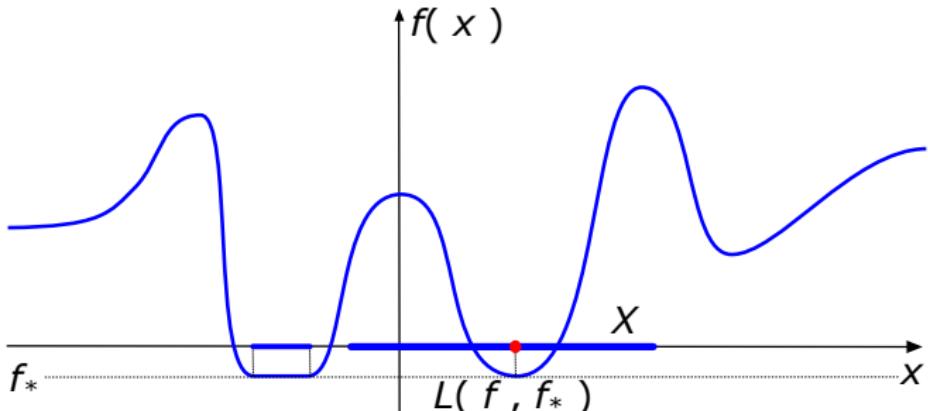
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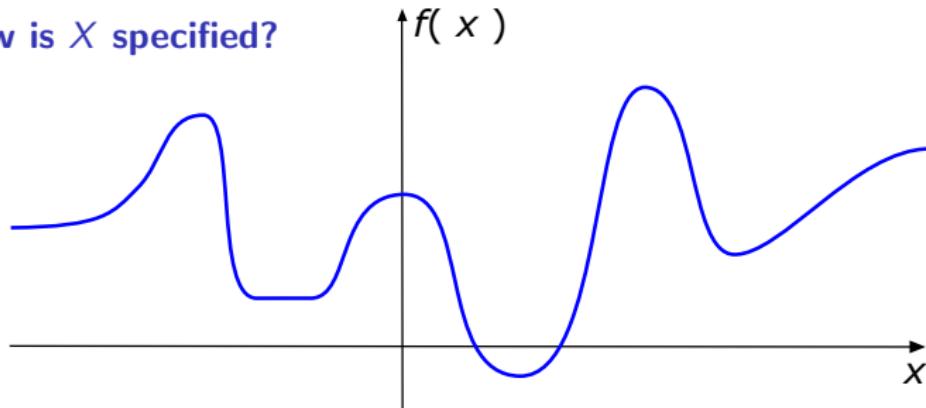
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- ▶ X can be “useless” (X_* same) or partly so (f_* same) \implies
makes sense to study the **unconstrained case $X = \mathbb{R}$** first

Anyhow, how is X specified?

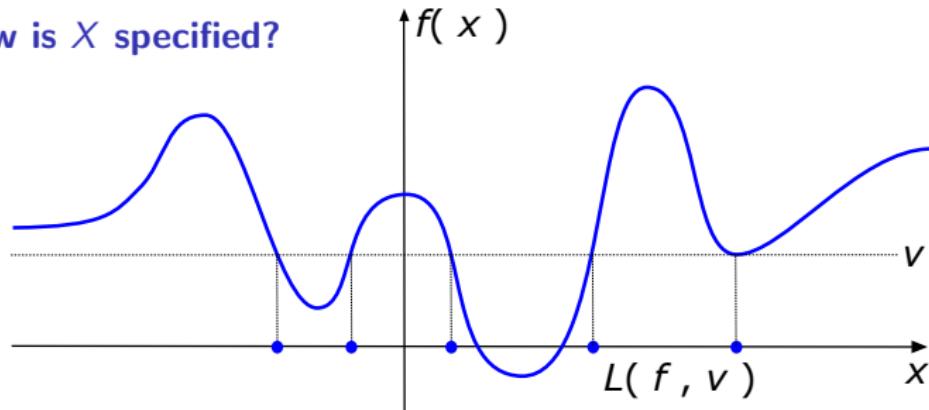
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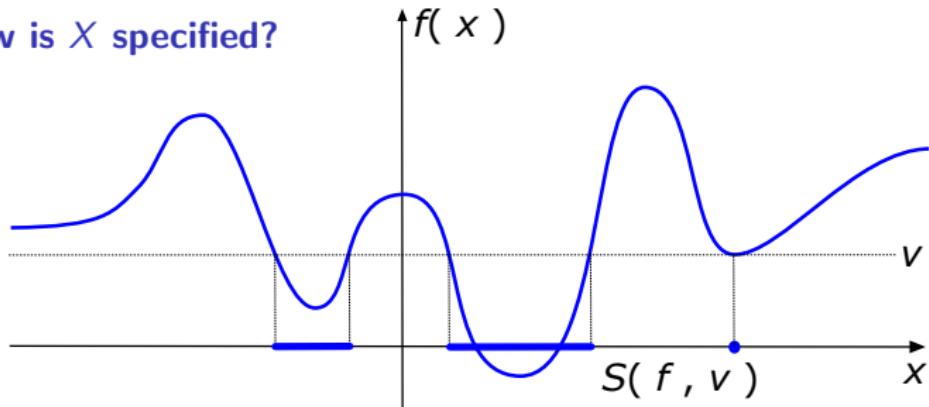
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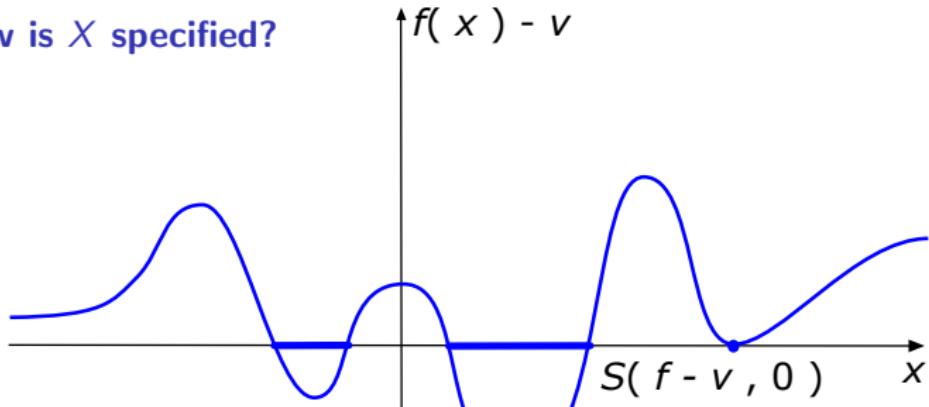
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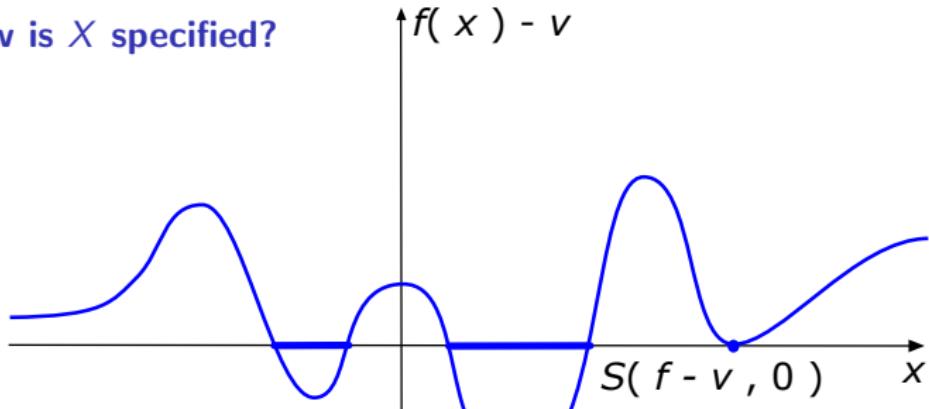
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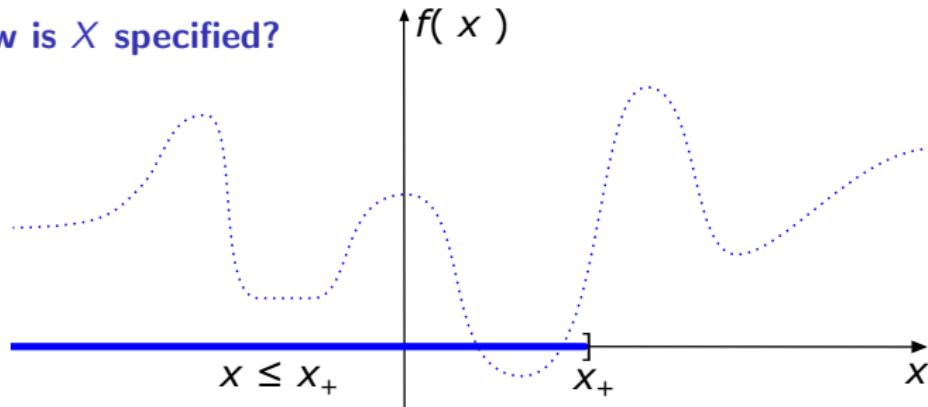
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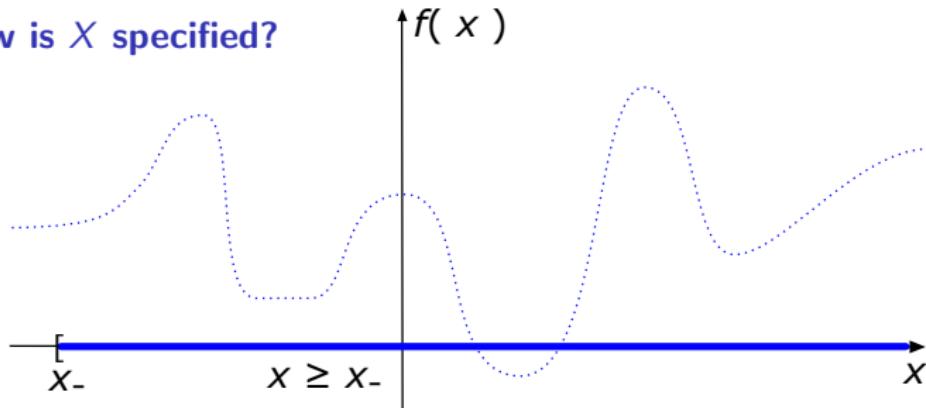
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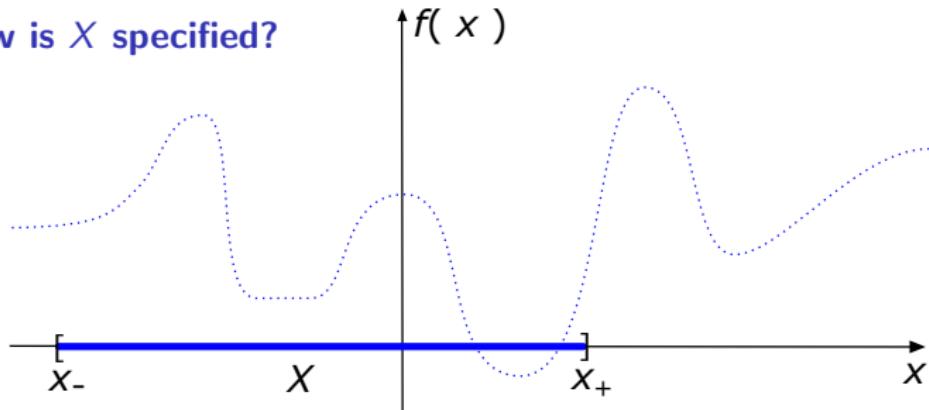
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- ▶ Simple and common: **bounds** $x \leq x_+$ (up)



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- ▶ Simple and common: **bounds** $x \leq x_+$ (up) / $x \geq x_-$ (dn),



- ▶ The “**abstract constraint** $x \in X$ ” need be specified somehow
- ▶ Often useful to represent a **set** via (more than) one **function(s)**
- ▶ Standard ways: **equality constraint** $g(x) = v \equiv X = \text{level set } L(g, v)$,
inequality constraint $g(x) \leq v \equiv \text{sublevel set } S(g, v) = \{x : g(x) \leq v\}$
- ▶ For convenience “ **v hidden in f** ” $\Rightarrow f(x) \leq 0, f(x) = 0$
- ▶ What if one rather wants $g(x) \geq 0$? Simply $-g(x) \leq 0$
- ▶ Usually **multiple constraints**: “ $g_1(x) \leq 0, g_2(x) \leq 0$ ” \equiv logical conjunction (“first condition **and** second condition”) \equiv **intersection** of (sub)level sets
- ▶ Simple and common: **bounds** $x \leq x_+$ (up) / $x \geq x_-$ (dn), **boxes** $x_- \leq x \leq x_+$

Outline

Optimization Problems

Optimization is difficult

Simple Functions, Univariate case

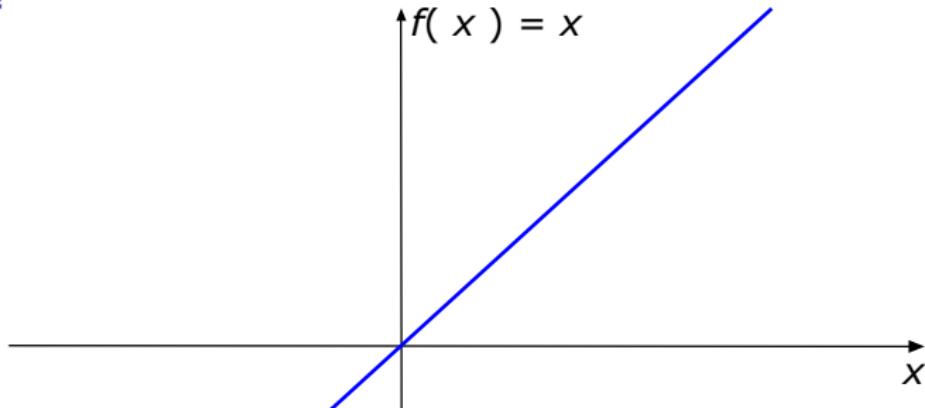
Simple Functions, Multivariate case

Multivariate Quadratic case: Gradient Method

Wrap up & References

Solutions

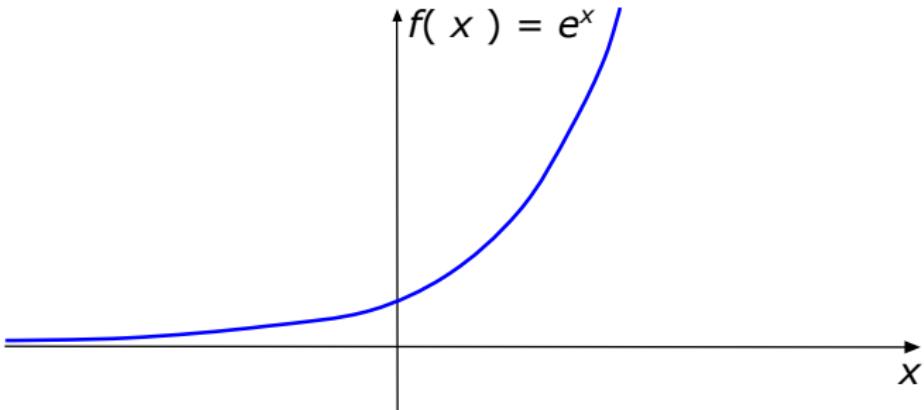
What if $f_* \nexists$?



- ▶ f has no minimum, (P) unbounded (below): $f_* = \nu(P) = -\infty$
- ▶ Just a convenient shorthand for $\forall t \in \mathbb{R} \exists x \in \mathbb{R}$ s.t. $f(x) \leq t$
i.e., “there is no (finite) lower bound on $\text{im}(f)$ ”
- ▶ Solving (P) actually (at least) two different things:
 - ▶ finding x_* and proving it is optimal (how??)
 - ▶ constructively proving f unbounded below (how??)
- ▶ Hardly ever happens in learning since $\mathcal{L}(w) \geq 0$
- ▶ Nontrivial and important in optimization (tied with duality, nonemptiness, . . .)

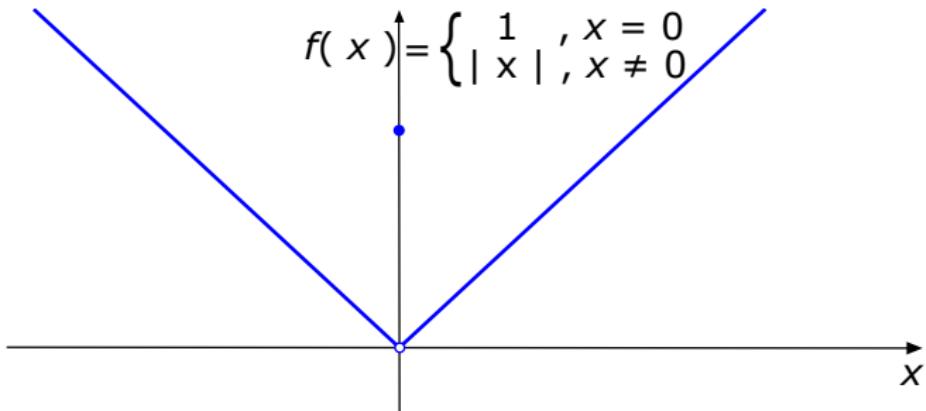
What if $f_* \exists$ but $x_* \nexists$?

7



- ▶ $\text{im}(f)$ is bounded below but has no minimum
- ▶ Either “naturally”

What if $f_* \exists$ but $x_* \nexists$?



- ▶ $\text{im}(f)$ is bounded below but has no minimum
- ▶ Either “naturally” or “forcibly”
- ▶ $\inf\{f(x) : x \in \mathbb{R}\} \exists$, but $\min\{f(x) : x \in \mathbb{R}\} \nexists$
- ▶ Arguably $f_* = \inf\{f(x) : x \in \mathbb{R}\}$, but $\nexists x_*$ s.t. $f_* = f(x_*)$
- ▶ $\text{im}(f)$ is **open**, does not contain its boundary (will see)

- \mathbb{R} totally ordered $\implies \forall x, y \in \mathbb{R}$, at least one among $x \leq y$, $y \leq x$ holds
- $S \subseteq \mathbb{R}$, $\underline{s} = \inf S \iff \underline{s} \leq s \ \forall s \in S \wedge \forall t > \underline{s} \exists s \in S \text{ s.t. } s \leq t$
 $\bar{s} = \sup S \iff \bar{s} \geq s \ \forall s \in S \wedge \forall t < \bar{s} \exists s \in S \text{ s.t. } s \geq t$
- $\underline{s} \in S \implies \underline{s} = \min S$, $\bar{s} \in S \implies \bar{s} = \max S$
- Issues: i) $\inf S / \sup S$ may not \exists in \mathbb{R} , ii) $\inf S / \sup S$ may not $\in S$
- Should write “ $\inf\{f(x)\dots\}$ ”, but we want (approximately) optimal solutions
- Set of extended reals: $\overline{\mathbb{R}} = \{-\infty\} \cup \mathbb{R} \cup \{+\infty\}$ (usually just \mathbb{R})
- For all $S \subseteq \mathbb{R}$, $\exists \sup / \inf S \in \overline{\mathbb{R}}$
- $\inf S = -\infty \iff \forall t \in \mathbb{R} \exists s \in S \text{ s.t. } s \leq t$
 $\sup S = +\infty \iff \forall t \in \mathbb{R} \exists s \in S \text{ s.t. } s \geq t$
just a convenient shorthand for “there is no (finite) inf / sup”
- $\inf \emptyset = \infty$, $\sup \emptyset = -\infty$

Is this a real problem in practice?

9

- ▶ Several ways to ensure this never happens (hypotheses on f , X)
- ▶ On computers " $x \in \mathbb{R}$ " typically is " $x \in \mathbb{Q}$ " with up to 16 digits precision
⇒ approximation errors unavoidable anyway
- ▶ Exact algebraic computation may be possible (if f is algebraic, which it may be not) but anyway usually too slow
- ▶ In fact learning going the opposite way (float, half, FP8, ...)
- ▶ Anyway, finding the exact x_* impossible in general [4, p. 408]
- ▶ For any fixed $\varepsilon > 0$, plenty of ε -approximate solutions (ε -optima):
 $x_\varepsilon \in \mathbb{R}$ s.t. $f_* \leq f(x_\varepsilon) \leq f_* + \varepsilon$
“as close to the optimal solution (value) as you want”
- ▶ Cost of solution algorithms typically depends on ε (sometimes very badly)
- ▶ And ε can't really become very small anyway (see above)

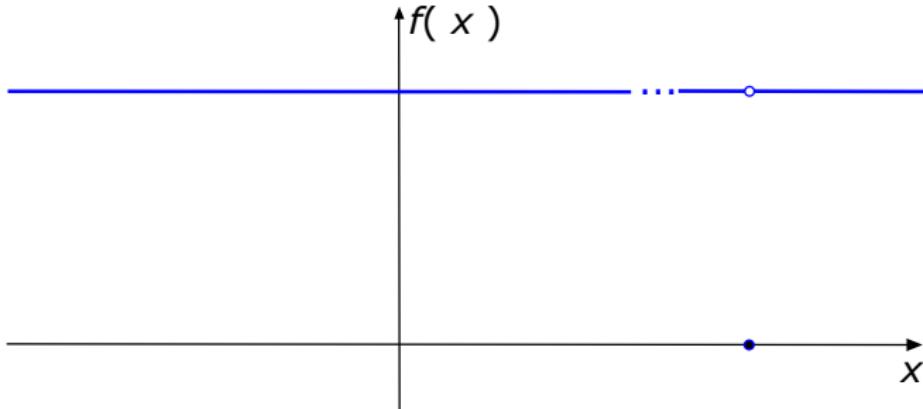
- Absolute gap: $A(x) = f(x) - f_*$ (≥ 0)
- Relative gap: $R(x) = (f(x) - f_*) / |f_*| = A(x) / |f_*|$ (≥ 0)
- Why $R(x)$? Because $\forall \alpha > 0$ $(P) \equiv (P_\alpha) \min\{\alpha f(x) : x \in \mathbb{R}\}$
 $\nu(P_\alpha) = \alpha f_* = \alpha \nu(P) \implies$ same $R(x)$ (scale invariant), different $A(x)$

Exercise: $R(x)$ ill-defined if $f_* = 0$, propose solutions & justify them (change f_*)

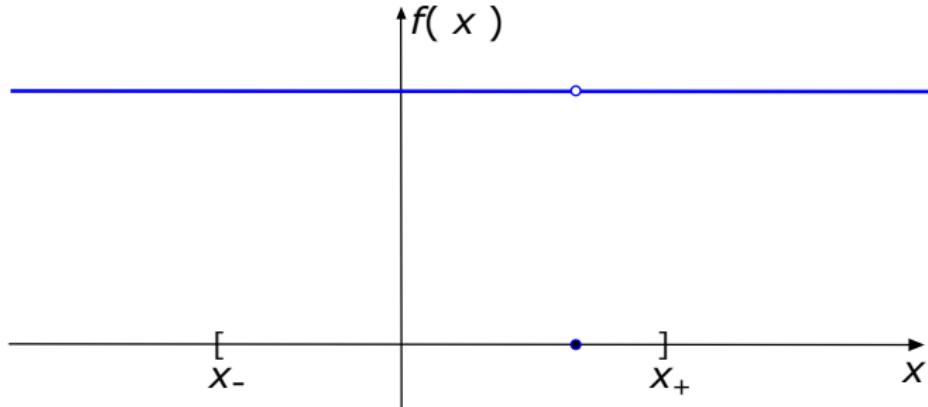
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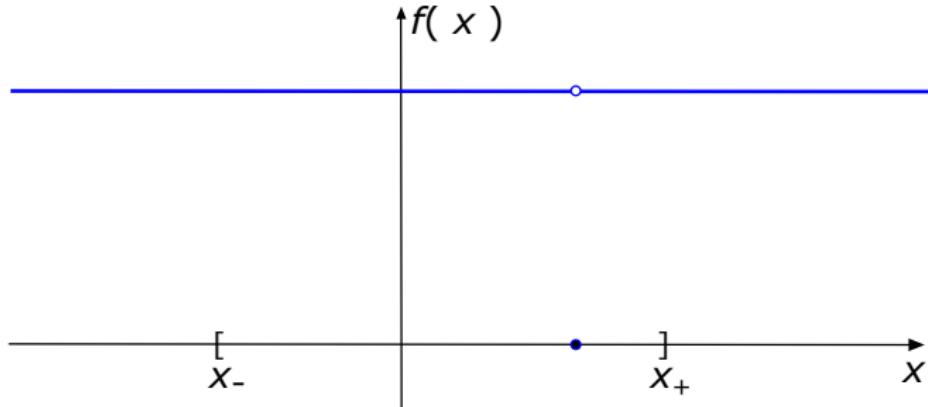
- ▶ (Approximately) solve (P) : fix ε , find x s.t. either $A(x) \leq \varepsilon$ or $R(x) \leq \varepsilon$
- ▶ Issue: computing $A(x)$ or $R(x)$ requires f_* which is typically unknown
- ▶ Could argue this is “the issue” in optimization: compute (an estimate of) f_*
- ▶ Sometimes \approx known in learning ($f_* \approx 0$ in NN, but not in SVM)
- ▶ A real issue only if global optimum x_* needed, hence not always



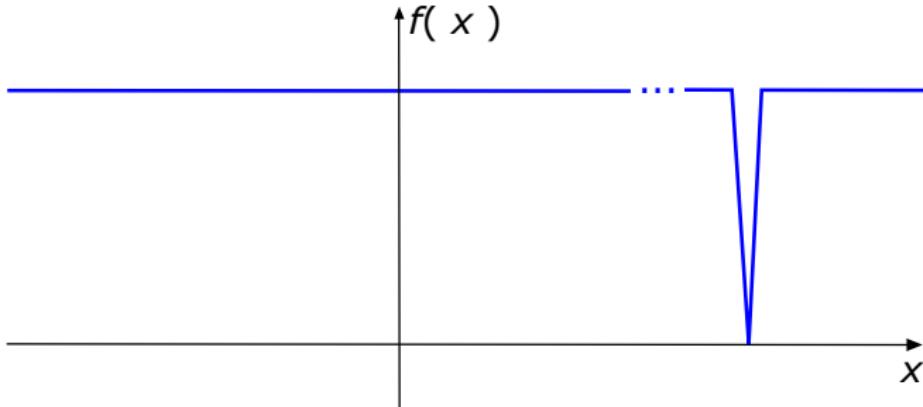
- Impossible because isolated minima can be anywhere [4, p. 408]



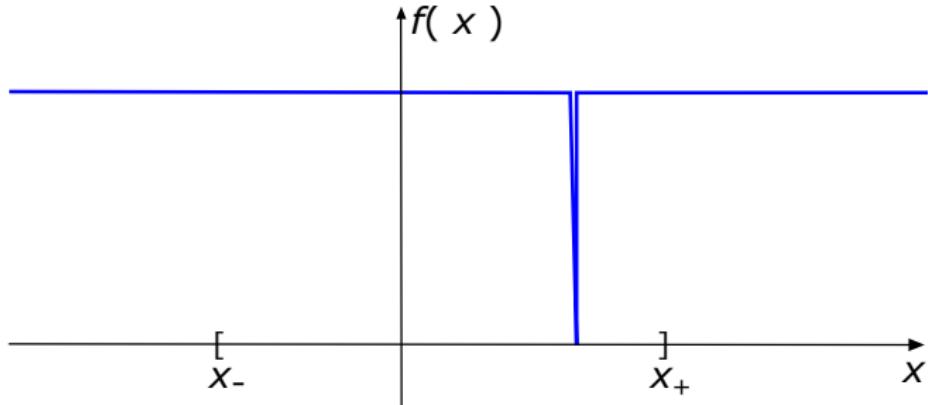
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- ▶ No: still uncountably many points to try



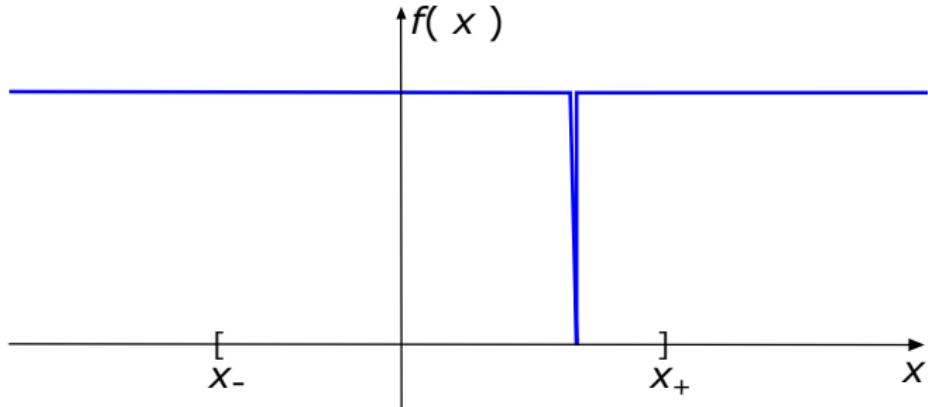
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- ▶ Is it because f “jumps”? No, f can have isolated ↓ spikes anywhere ... even on $X = [x_-, x_+]$ as spikes can be arbitrarily narrow
- ▶ To make (even approximate) optimization even possible, f must be “nice”
- ▶ Let's start with the **nicest possible ones** where optimization is (\approx) trivial

Outline

Optimization Problems

Optimization is difficult

Simple Functions, Univariate case

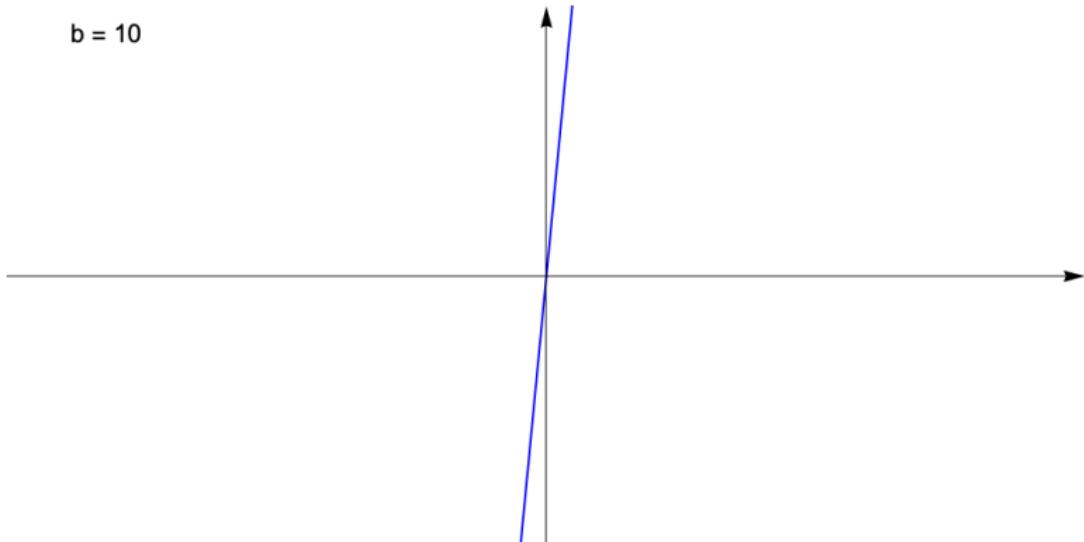
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Wrap up & References

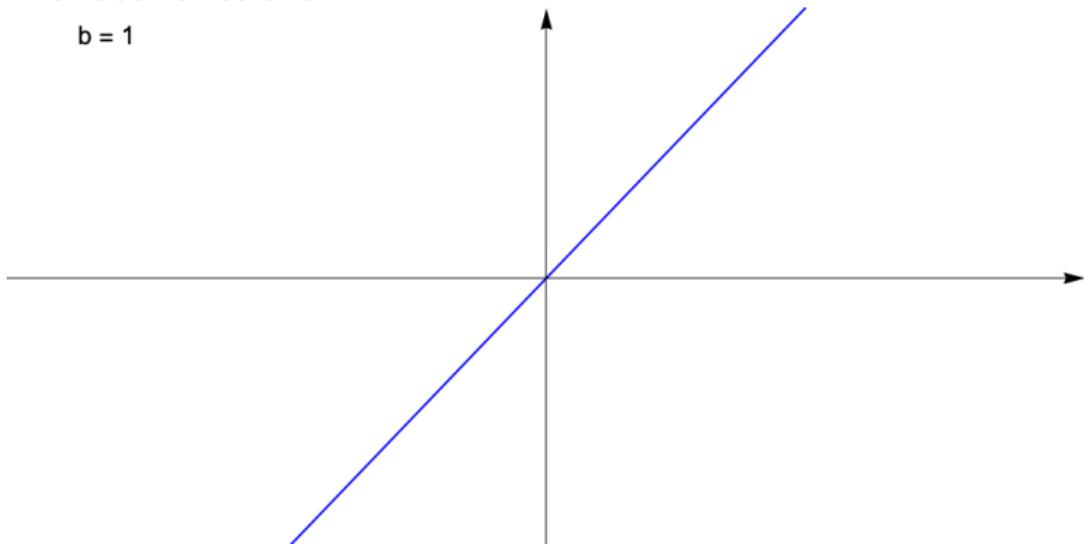
Solutions

$$b = 10$$



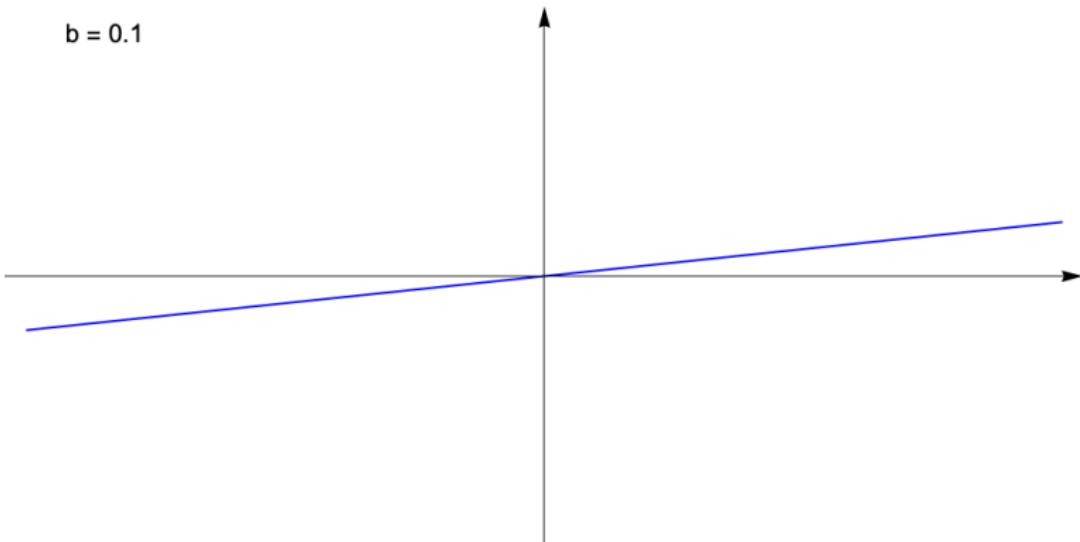
- ▶ The simplest possible function: $f(x) = bx$ (linear), fixed $b \in \mathbb{R}$
- ▶ As many different functions as real numbers (bijection)
- ▶ $b > 0 \equiv$ increasing: $x > z \implies f(x) > f(z)$

$$b = 1$$



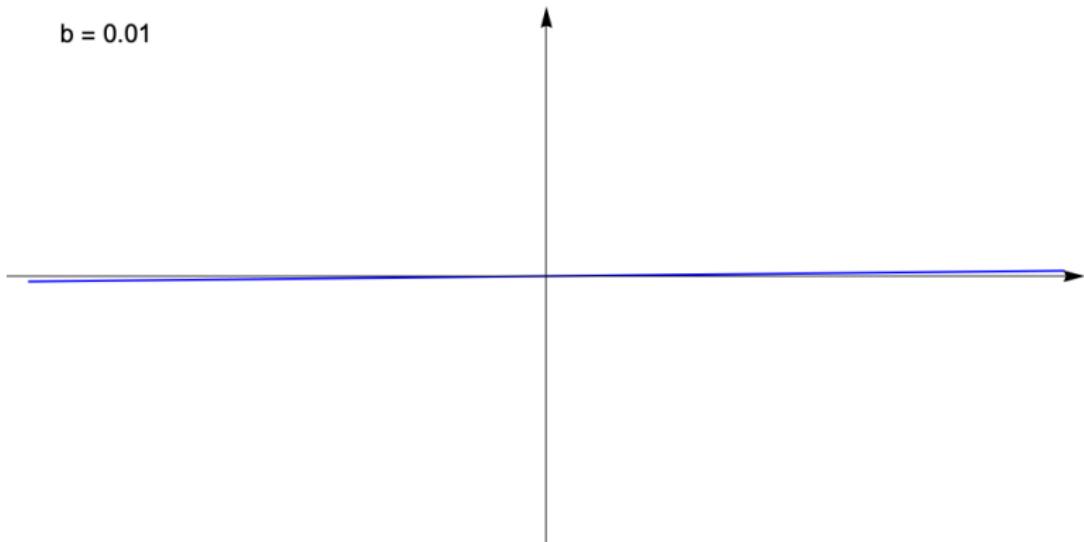
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$$b = 0.1$$



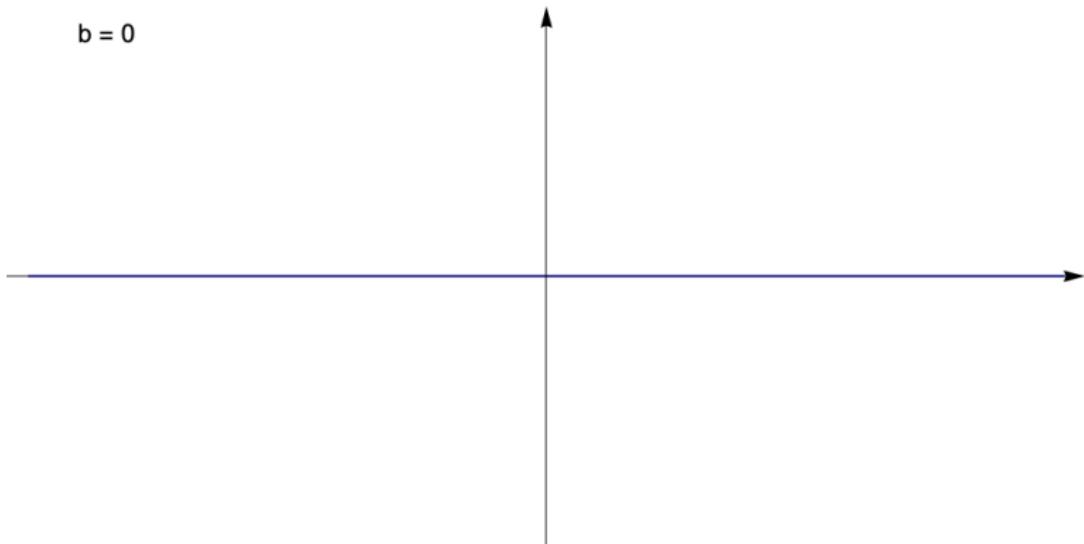
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$$b = 0.01$$



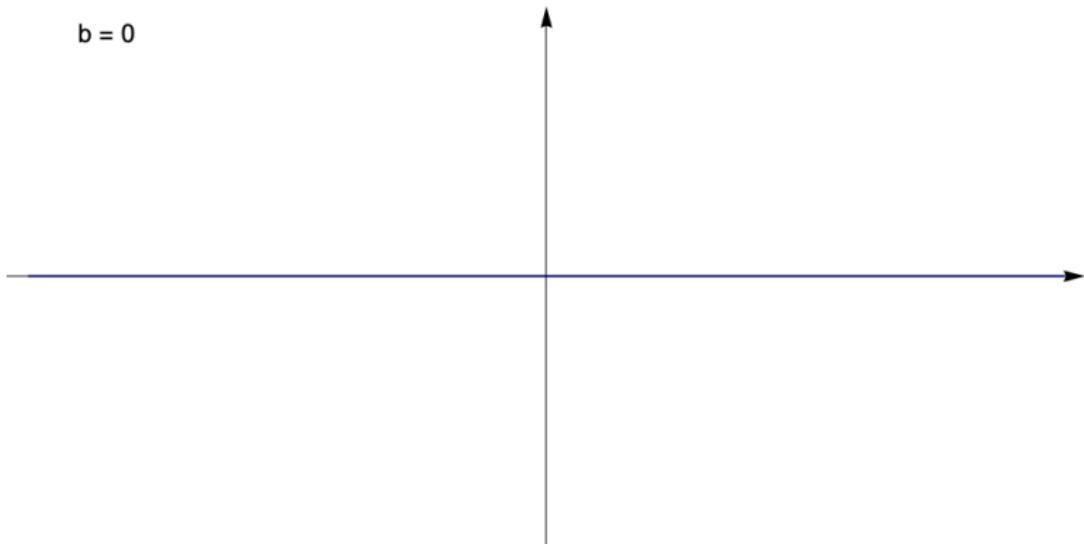
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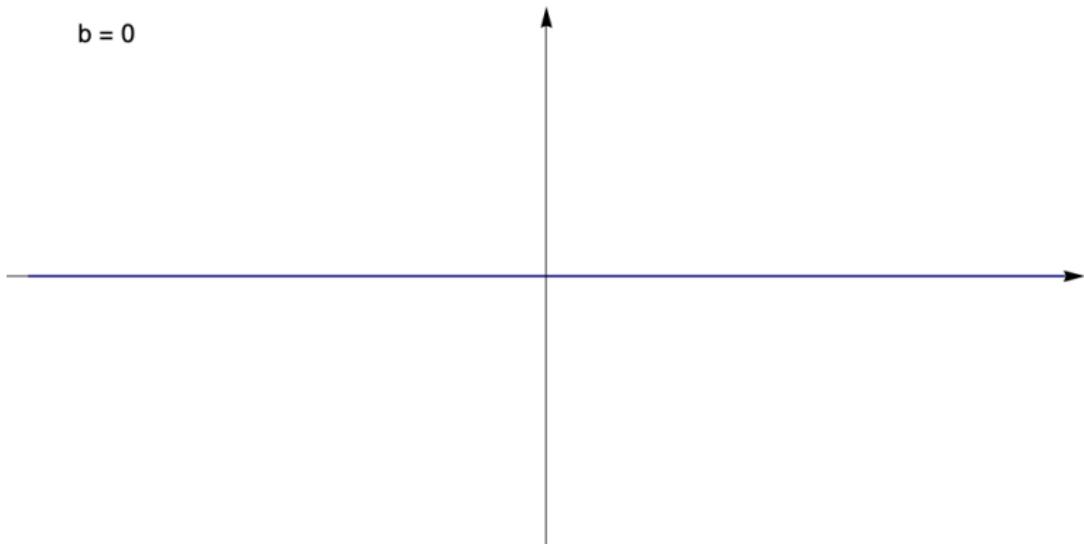
- ▶ The simplest possible function: $f(x) = bx$ (linear), fixed $b \in \mathbb{R}$
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$$b = 0$$



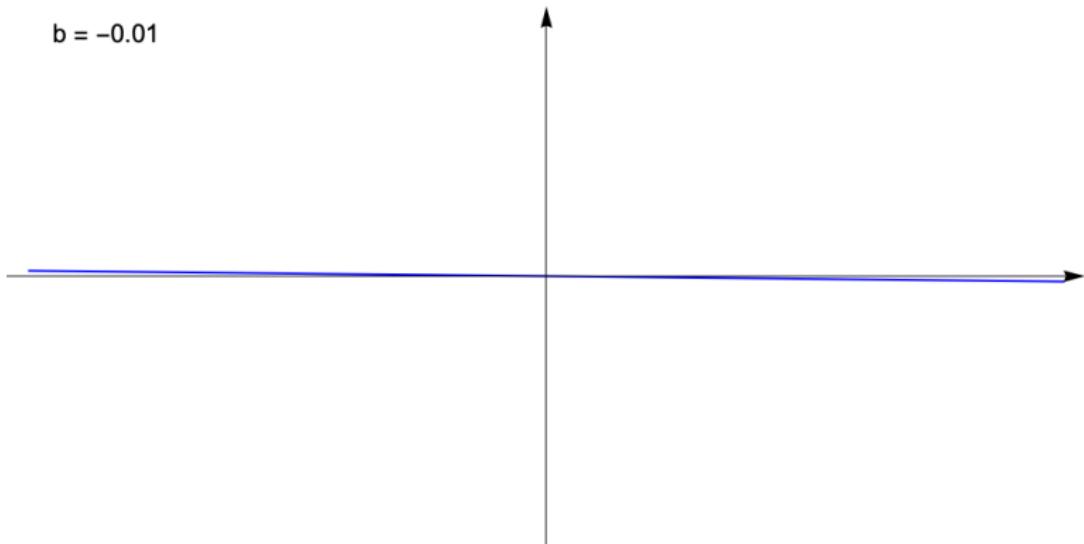
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$$b = 0$$



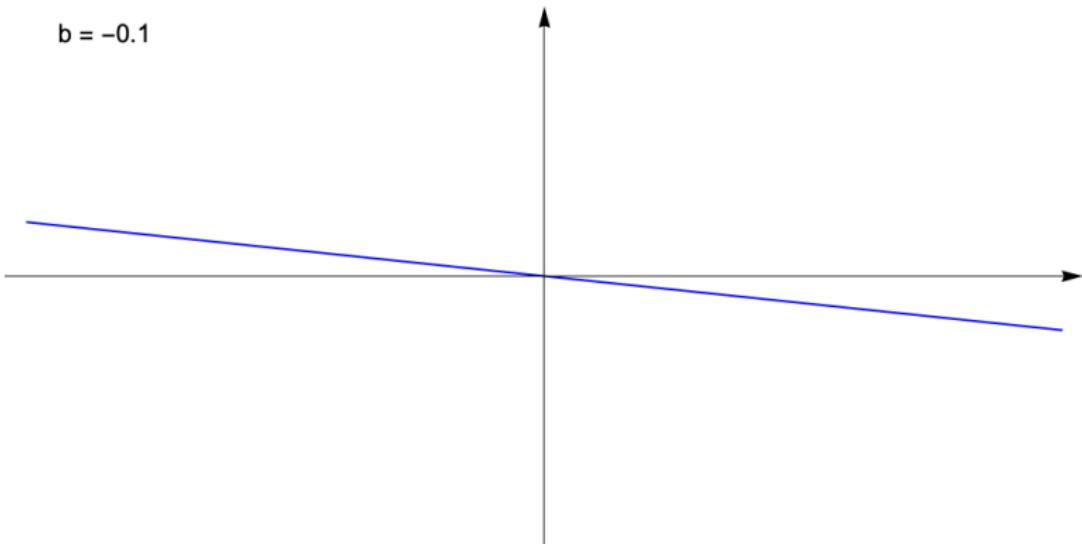
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$$b = -0.01$$

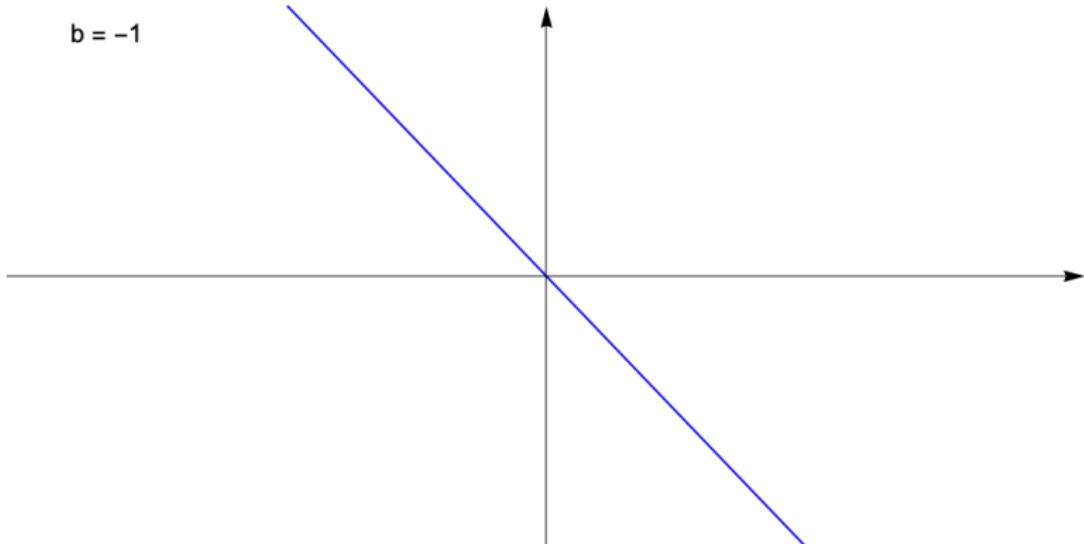


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$$b = -0.1$$

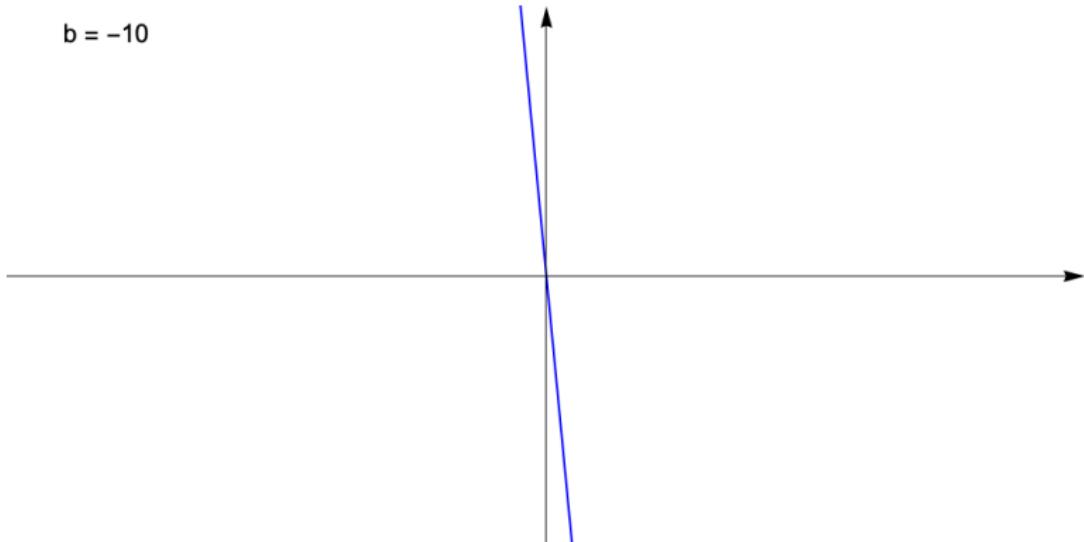


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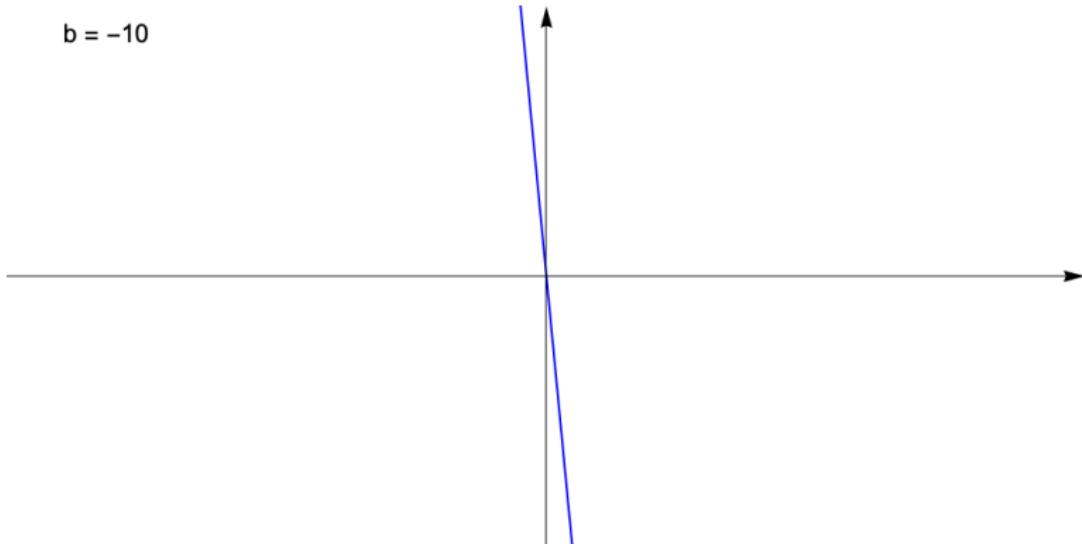
$$b = -10$$



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Exercise: Formally prove the stated properties

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Exercise: Formally prove the stated properties

- ▶ $b =$ linear coefficient = **slope**: the larger $|b|$, the steeper the line

- ▶ Too easy: $\min = -\infty$, $\max = +\infty$ unless $b = 0 \implies \min = \max = 0$
- ▶ More interesting: [box-constrained optimization](#)

$$(P) \quad \min\{f(x) : x \in [x_-, x_+]\}$$

with $-\infty \leq x_- \leq x_+ \leq +\infty \equiv X$ possibly (half-)infinite interval

- ▶ [Constraints often useful](#), (finite) box constraints (very simple) especially so
- ▶ $b > 0 \implies \operatorname{argmin} = x_-, \min = f(x_-), \operatorname{argmax} = x_+, \max = f(x_+)$
- ▶ “Works” even if $x_- = -\infty$ and/or $x_+ = +\infty$, as $b \cdot (\pm\infty) = \pm\infty$

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- ▶ [Closed formula \$O\(1\)\$, don't get used to it](#)
- ▶ Yet [solving simple problems](#) the basis of solving complicated ones

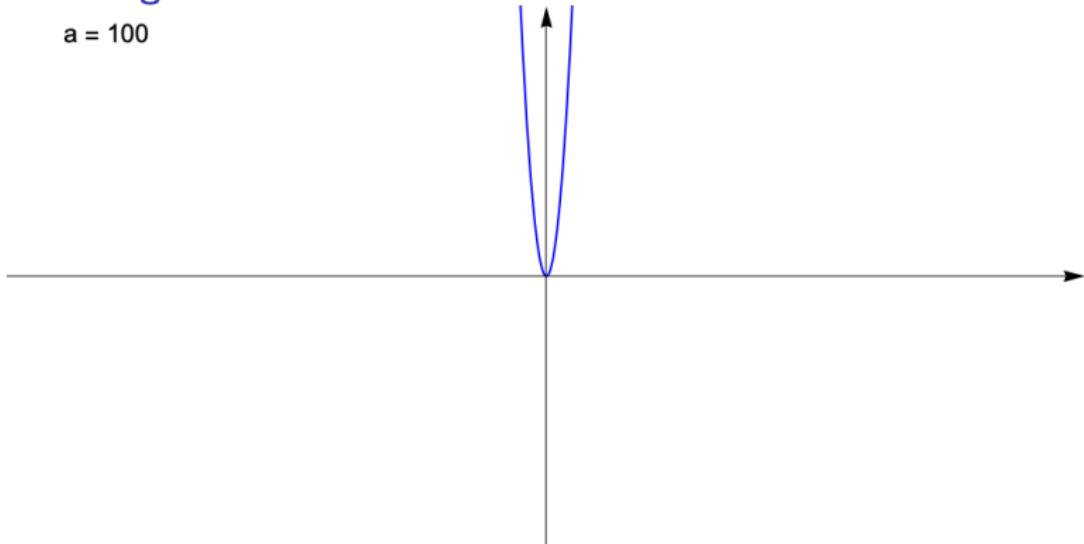
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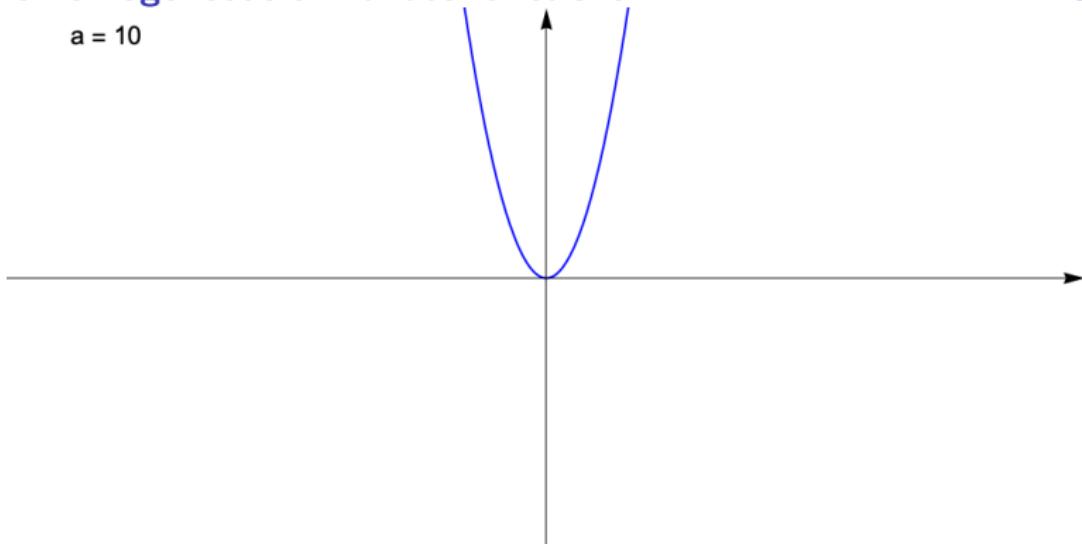
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⇒ cannot be chosen/measured to ∞ precision
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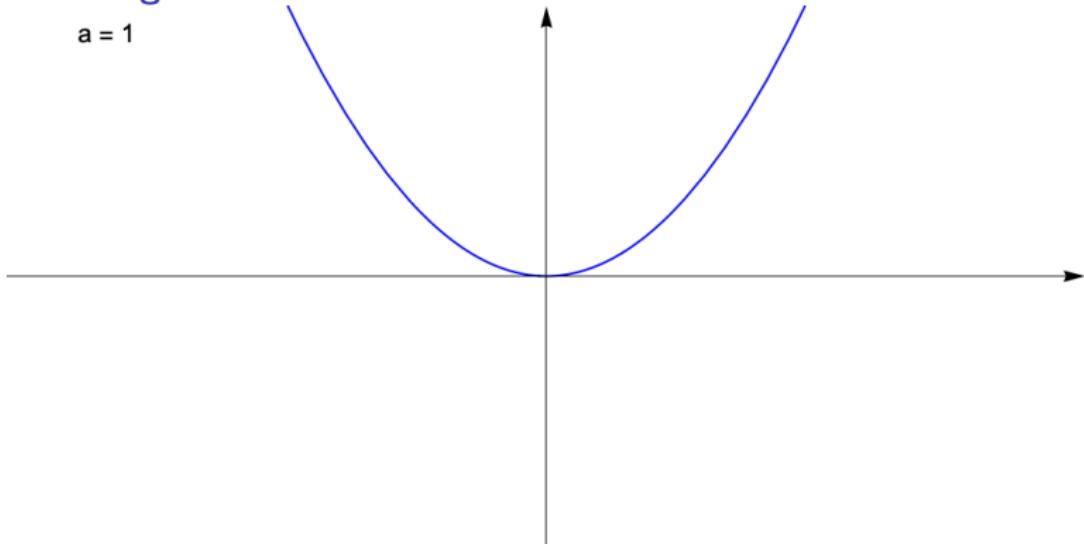
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again, plenty of ε -optimal solutions however chosen $\varepsilon > 0$
- ▶ Does it make any sense at all? Hardly: if x_-, x_+ “can't be touched”, use
 $X = [x_- + \varepsilon_-, x_+ - \varepsilon_+]$ for appropriately chosen ε_\pm
- ▶ All in all? Just use closed intervals and be done with it
- ▶ Will generalise to “just use closed sets and be done with it”

$a = 100$ 

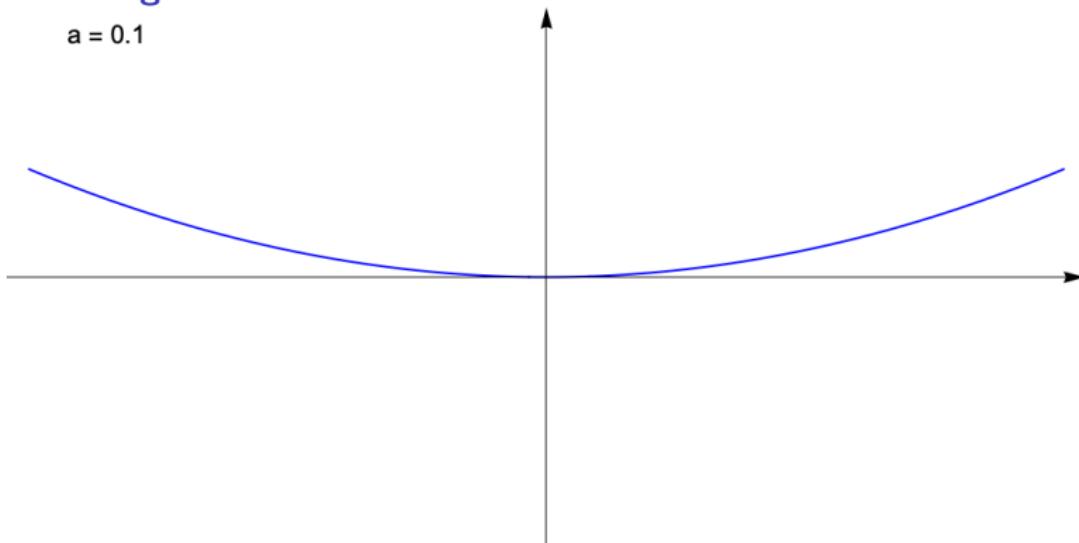
- ▶ Next simplest function: $f(x) = ax^2$ (homogeneous quadratic), **fixed $a \in \mathbb{R}$**
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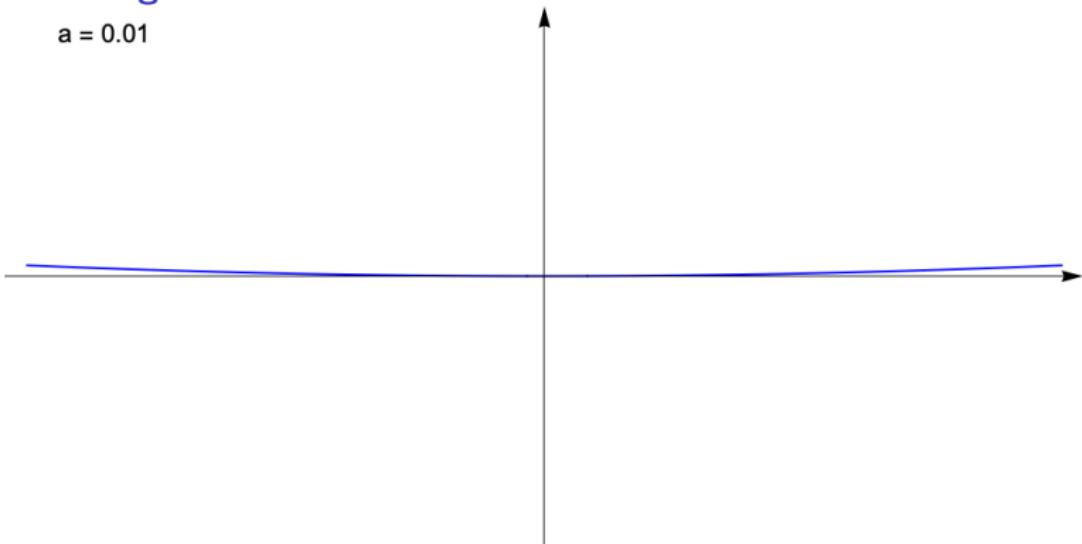


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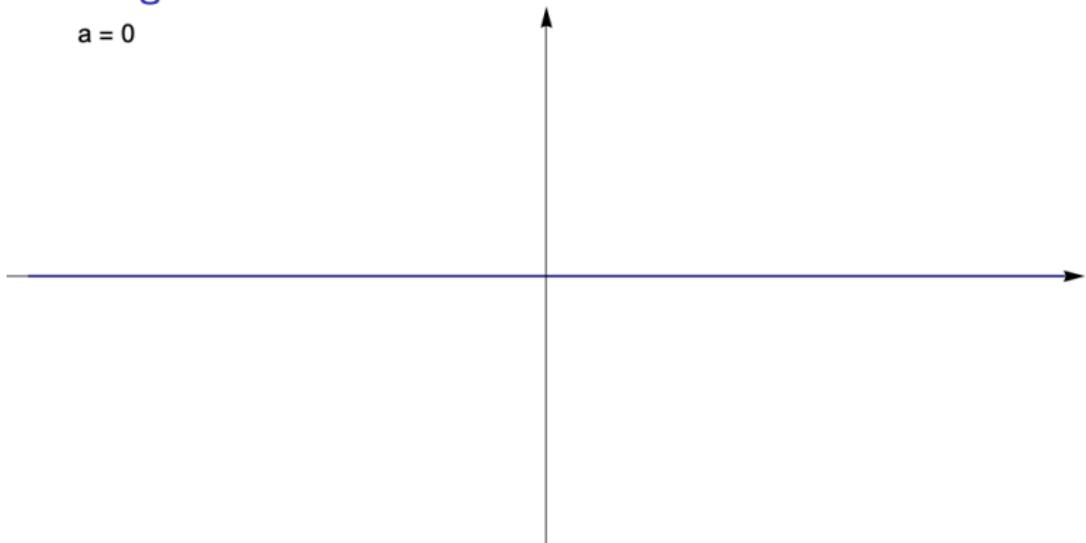


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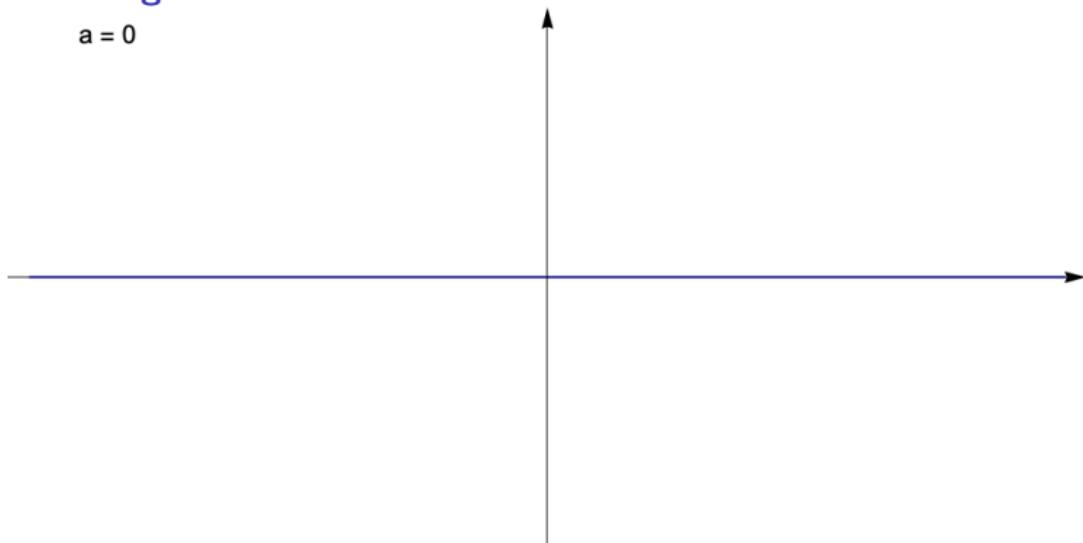
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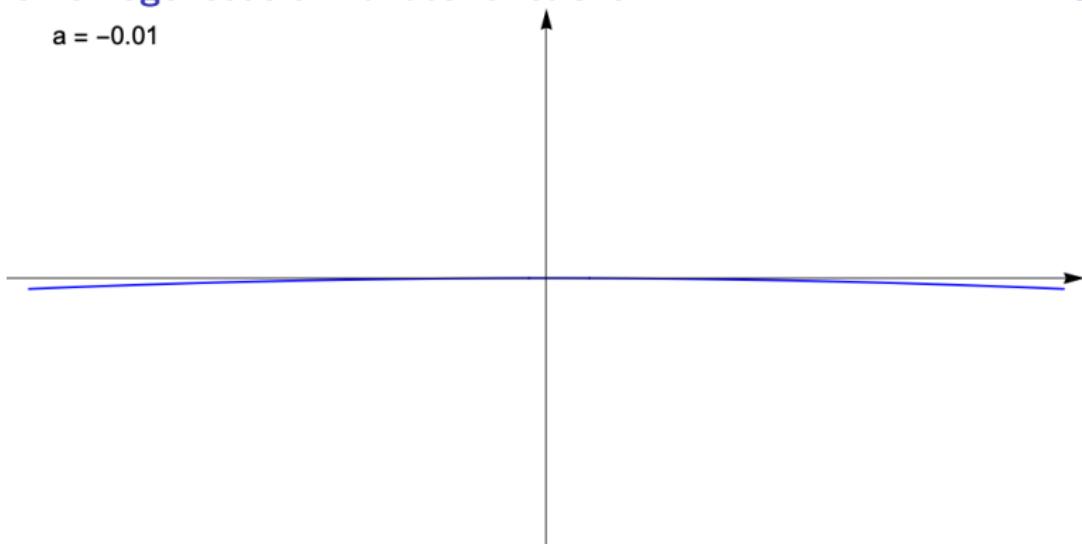


- ▶ Next simplest function: $f(x) = ax^2$ (homogeneous quadratic), fixed $a \in \mathbb{R}$
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- ▶ $a = 0 \equiv$ nonincreasing for $x \leq 0$, nondecreasing for $x \geq 0$ and

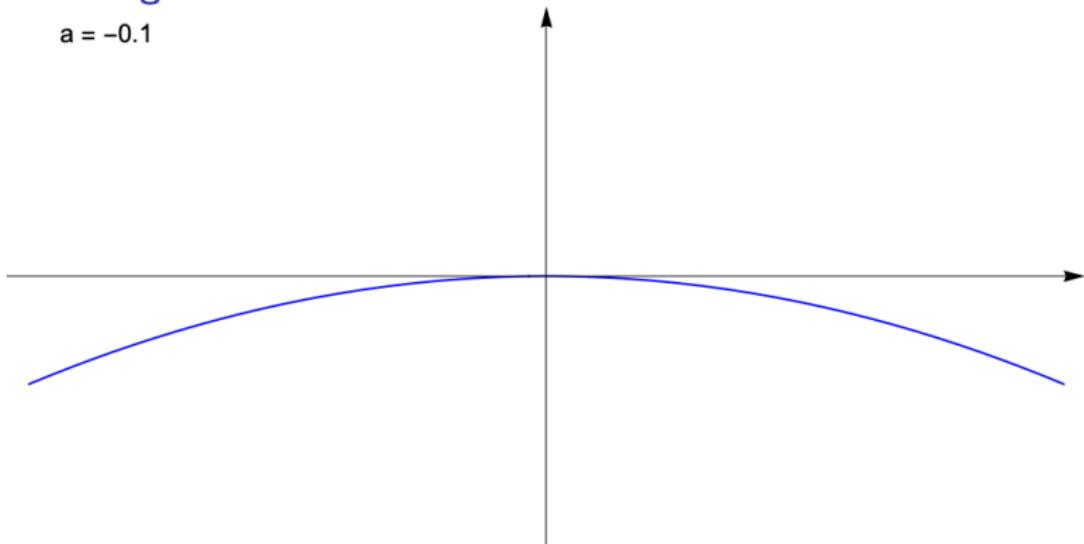


- ▶ Next simplest function: $f(x) = ax^2$ (homogeneous quadratic), fixed $a \in \mathbb{R}$
- ▶ As many different functions as real numbers (bijection)
- ▶ $a = 0 \equiv$ nondecreasing for $x \leq 0$, nonincreasing for $x \geq 0$ (constant)

$$a = -0.01$$

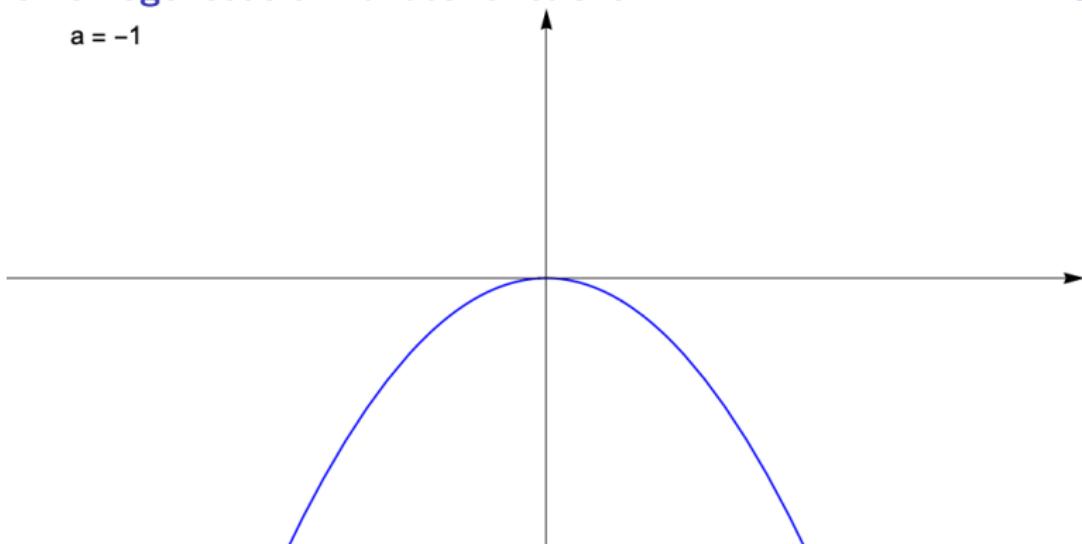


- ▶ Next simplest function: $f(x) = ax^2$ (homogeneous quadratic), fixed $a \in \mathbb{R}$
- ▶ As many different functions as real numbers (bijection)
- ▶ $a < 0 \equiv$ increasing for $x \leq 0$, decreasing for $x \geq 0$

$a = -0.1$ 

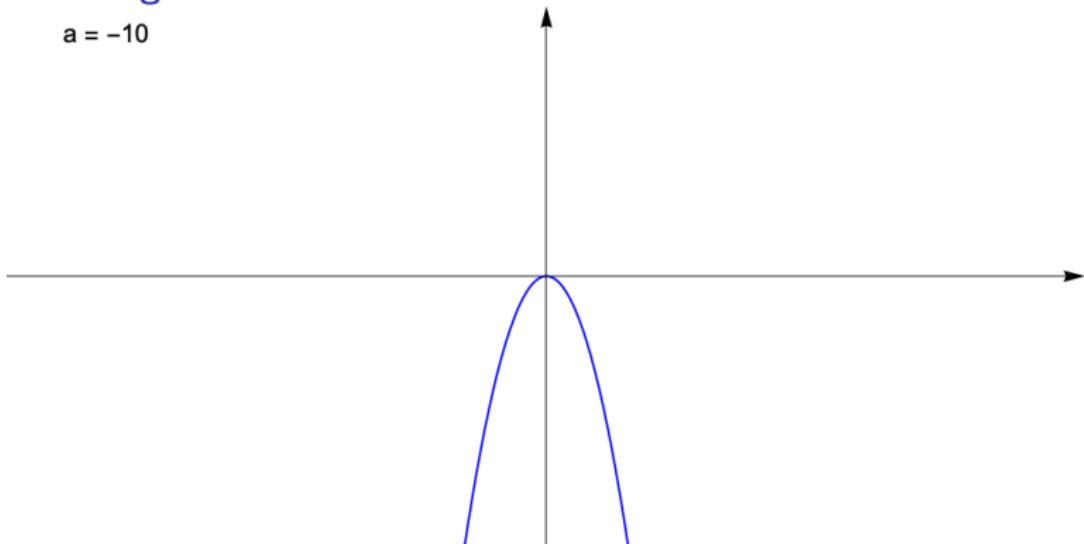
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$$a = -1$$



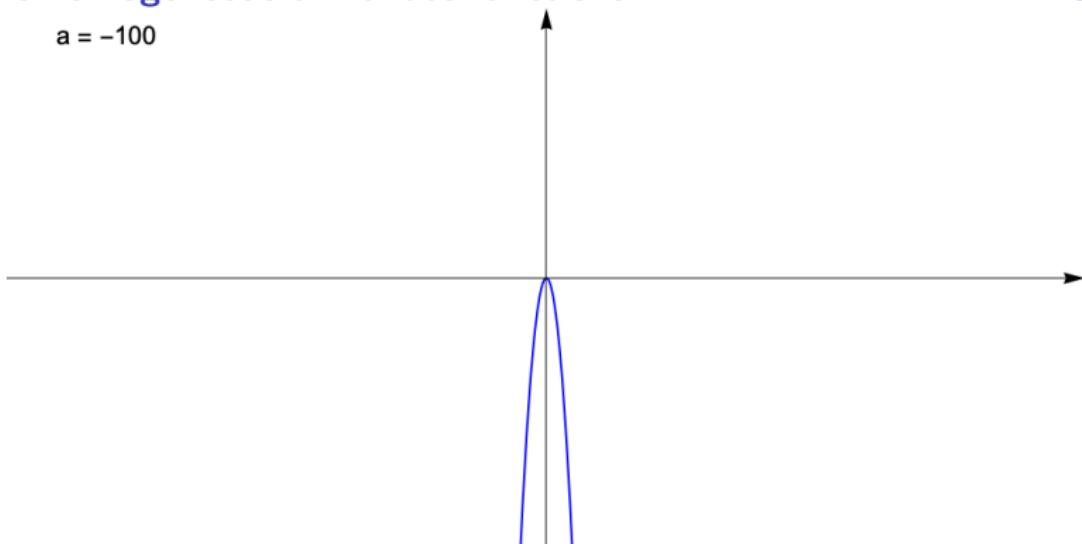
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$$a = -10$$



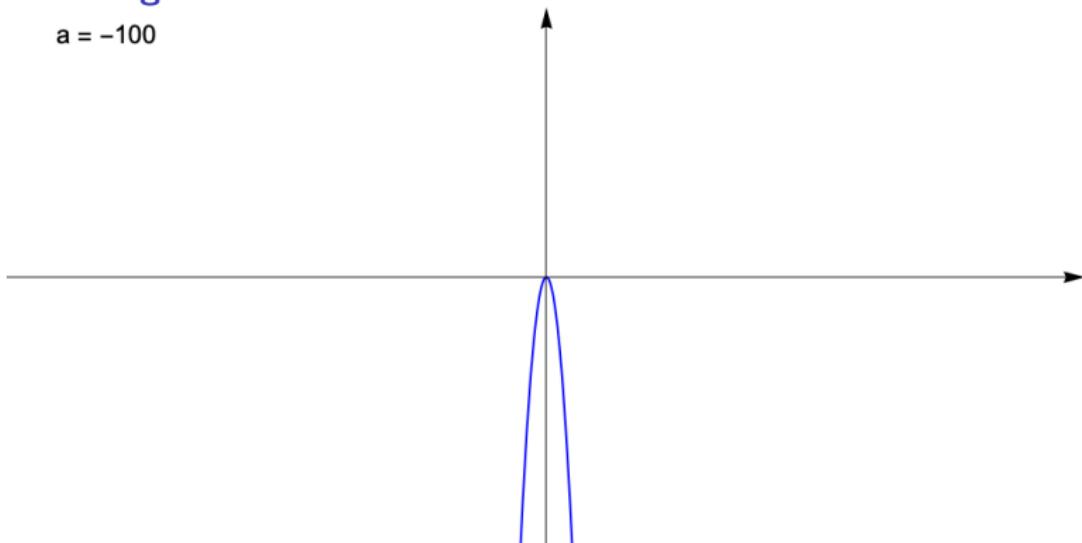
- ▶ Next simplest function: $f(x) = ax^2$ (homogeneous quadratic), fixed $a \in \mathbb{R}$
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$$a = -100$$



- ▶ Next simplest function: $f(x) = ax^2$ (homogeneous quadratic), fixed $a \in \mathbb{R}$
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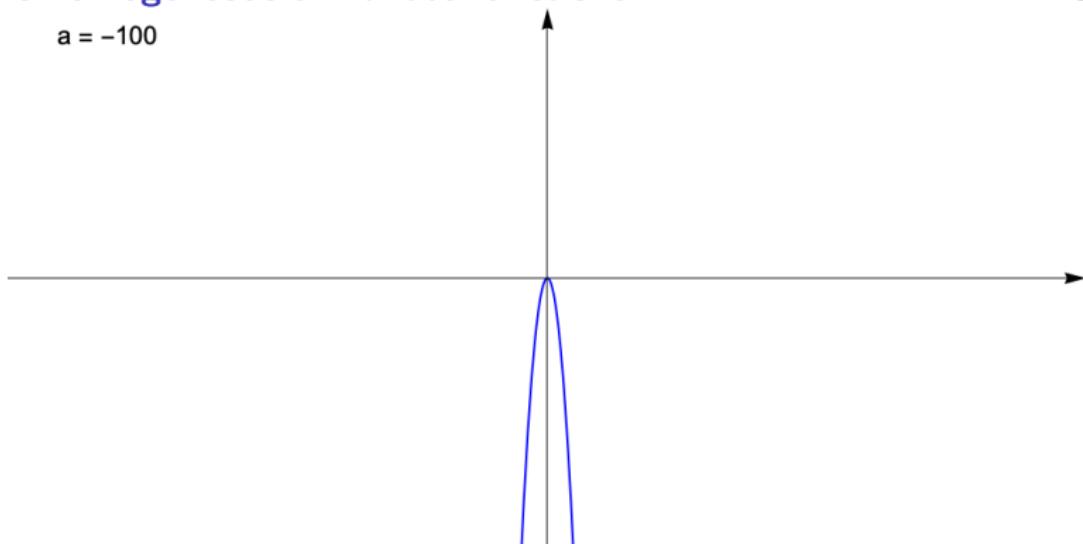
$$a = -100$$



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Exercise: Formally prove the stated properties

$$a = -100$$



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Exercise: Formally prove the stated properties

- ▶ $a =$ quadratic coefficient = **curvature**: the larger $|a|$, the steeper the parabola

- ▶ Clearly depends (and symmetric) on sign of a :
 - ▶ $a > 0 \implies \min = \text{argmin} = 0, \max = +\infty, \text{argmax} = \pm\infty$
 - ▶ $a < 0 \implies \max = \text{argmax} = 0, \min = -\infty, \text{argmin} = \pm\infty$
- ▶ Box-constrained optimization on (closed) $X = [x_-, x_+]$ more interesting
- ▶ $a > 0 \implies$ three cases
 - ▶ $x_+ < 0 \implies \text{argmin} = x_+, \text{argmax} = x_-$
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Exercise: Formally prove the result, state & prove cases $a < 0$ and $a = 0$

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Exercise: Formally prove the result, state & prove cases $a < 0$ and $a = 0$

- ▶ Again closed formula $O(1)$, don't get used to it
- ▶ $\max\{f(x)\}$ and $\min\{f(x)\}$ somewhat \neq (cf. last case), will see much more

- ▶ Next step: $f(x) = ax^2 + bx$ (non-homogeneous quadratic), fixed $(a, b) \in \mathbb{R}^2$
- ▶ As many different functions as pairs of real numbers (bijection)
- ▶ Basically, a homogeneous quadratic + a linear
- ▶ However, $\min\{ax^2 + bx\} \neq \min\{ax^2\} + \min\{bx\}$
- ▶ 0 clearly always a root, but in general not the argmin / argmax
- ▶ Powerful general concept: if $f(x)$ is “too complicated”, make it “simpler”
- ▶ Sometimes this can be done by changing the space of variables (reformulation)
- ▶ In this case: change the input space so that it becomes homogeneous
- ▶ Clearly only needed if both $a \neq 0$ and $b \neq 0$

- ▶ Fundamental trick: $\bar{x} = -b/2a$ (because I say so), $z = x - \bar{x} \equiv x = z + \bar{x}$
- ▶ The z -space is the x -space where the origin is moved to \bar{x}
- ▶ Just algebra: $f(x) = a(z + \bar{x})^2 + b(z + \bar{x}) = az^2 + 2az\bar{x} + a\bar{x}^2 + bz + b\bar{x}$
 $= az^2 + (2a\bar{x} + b)z + [a\bar{x}^2 + b\bar{x}] = az^2 + f(\bar{x}) = g(z)$ [$2a\bar{x} + b = 0$]
- ▶ Translated by \bar{x} horizontally (and by $f(\bar{x})$ vertically), $f(x)$ is homogeneous
- ▶ Its argmin / argmax (depending on sign of a) is $z = 0 \equiv x = \bar{x}$
- ▶ Then, just ▶ Optimizing a quadratic homogeneous function for $g(z)$
- ▶ Yet again, closed formula $O(1)$, don't get used to it

Exercise: Flesh out the details: describe all cases in terms of f and x

Exercise: Discuss the position of \bar{x} and the roots of f depending on a, b

Outline

Optimization Problems

Optimization is difficult

Simple Functions, Univariate case

Simple Functions, Multivariate case

Multivariate Quadratic case: Gradient Method

Wrap up & References

Solutions

- ▶ Next crucial step: $f : \mathbb{R}^n \rightarrow \mathbb{R}$, i.e., $f(x_1, x_2, \dots, x_n) = f(\mathbf{x})$
with $\mathbf{x} = [x_i]_{i=1}^n = [x_1, x_2, \dots, x_n] \in \mathbb{R}^n$
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(hyperrectangle) $X = \{x \in \mathbb{R}^n : x_- \leq x \leq x_+\}$, $x_\pm \in \mathbb{R}^n$ (with $x_- \leq x_+$)
- ▶ Assume $x_- = 0$, $x_+ = u = [1, \dots, 1]$ and we can **only look to integer values**:
still have 2^n points to look at (binary hypercube), grows too fast with n

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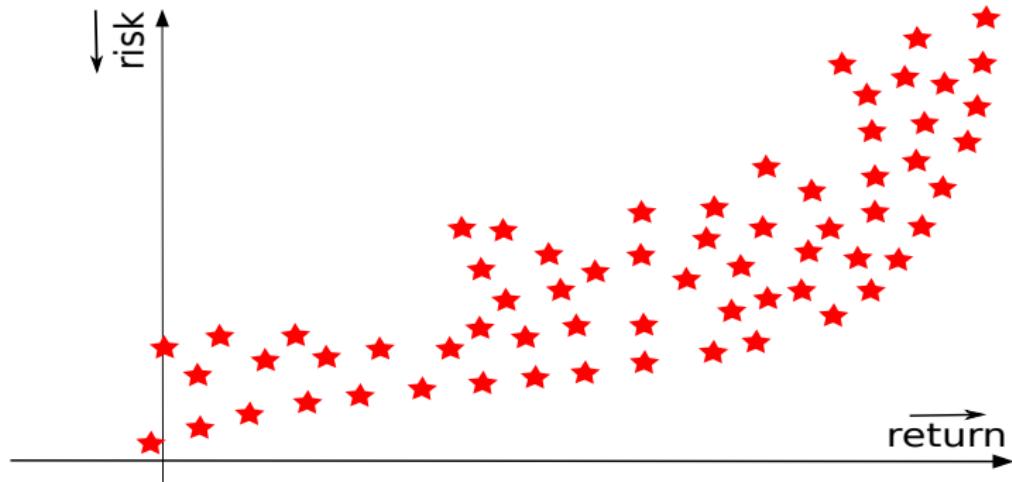
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still have 2^n **points to look at** (binary hypercube), grows too fast with n
- ▶ Even picturing things is more complex and **requires appropriate tools**

- ▶ Already “ $f : X \rightarrow \mathbb{R}$ ” a **rather strong assumption**:
can “express all the value of any $x \in X$ with a single number” \implies
given x' and x'' I can always tell which one I like best (\mathbb{R} has **total order**)
- ▶ Often there would be **more than one objective**:

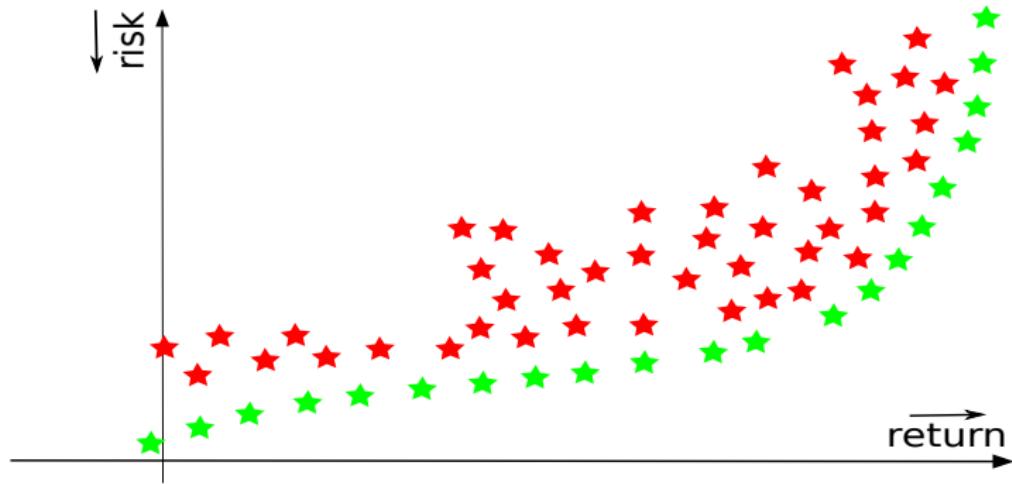
$$(P) \quad \min \{ [f_1(x), f_2(x), \dots] : x \in X \}$$

with f_1, f_2, \dots **contrasting** and/or with **incomparable units** (apples vs. oranges)

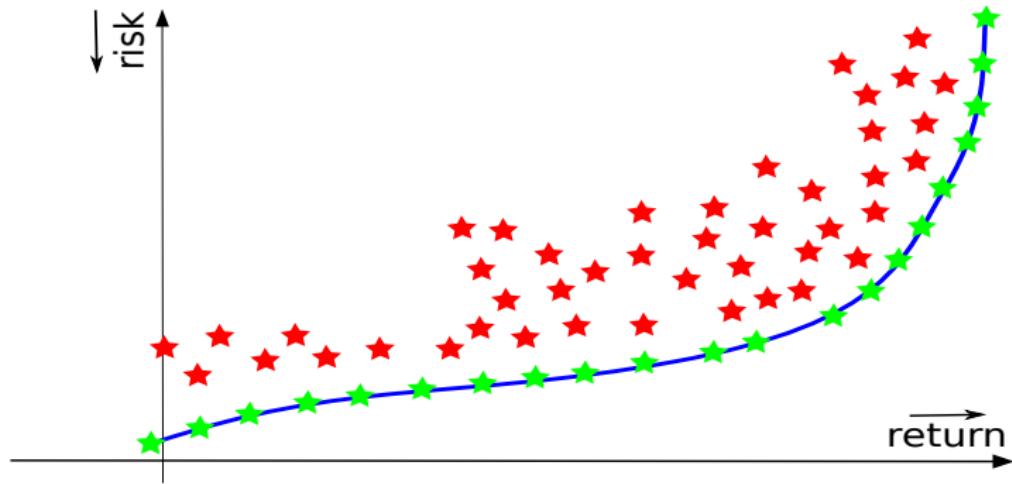
- ▶ car cost vs. flashiness vs. km/l vs. # seats vs. trunk space ...
- ▶ loss function $\mathcal{L}(w)$ vs. regularity $R(w)$ in ML
- ▶ ...
- ▶ Vector-valued (a.k.a. **multi-objective**) optimization: $f : X \rightarrow \mathbb{R}^k$ with $k > 1$
- ▶ Textbook example: portfolio selection problem
 - ▶ $X =$ set of financial instruments portfolios available to buy
 - ▶ $f_1(x) =$ expected return of portfolio x (€)
 - ▶ $f_2(x) =$ risk of portfolio x not achieving the expected return (%), CVAR, ...)



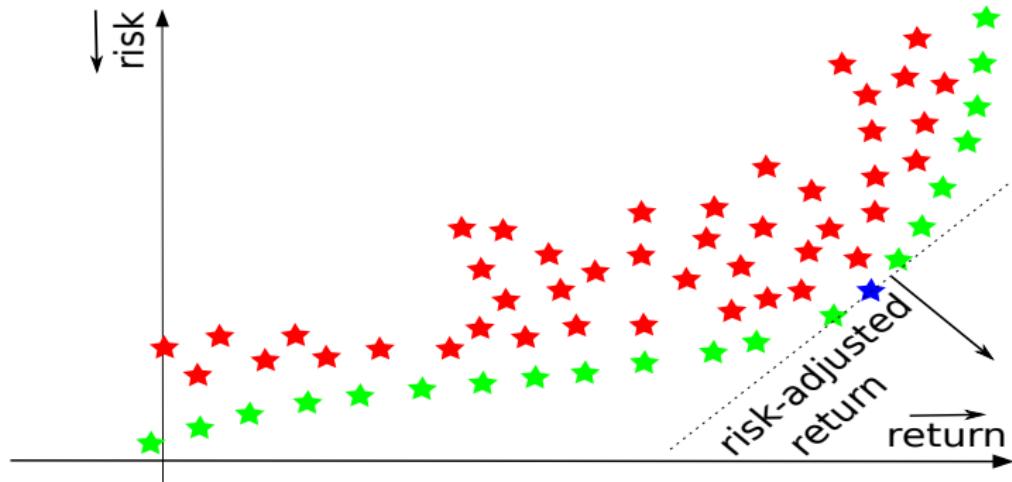
- ▶ \mathbb{R}^k with $k > 1$ has no total order \implies no “best” solution, only



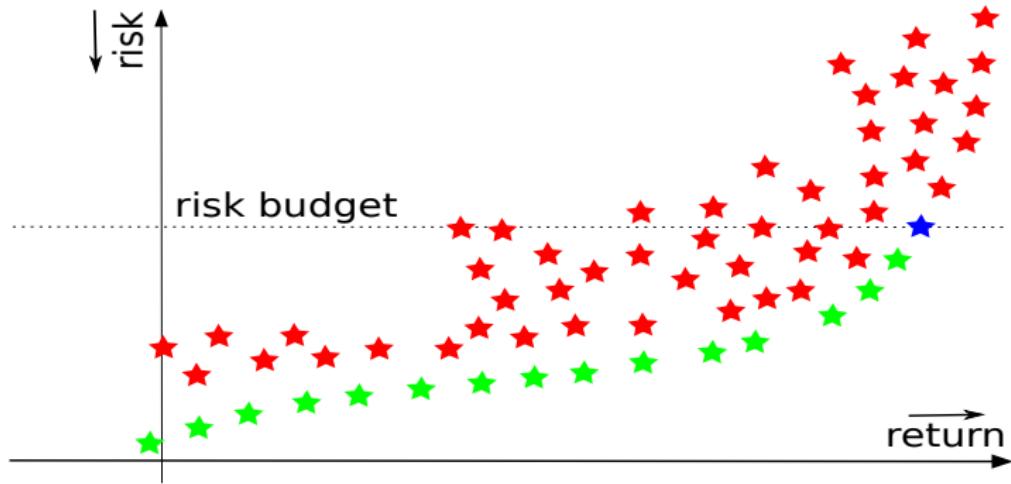
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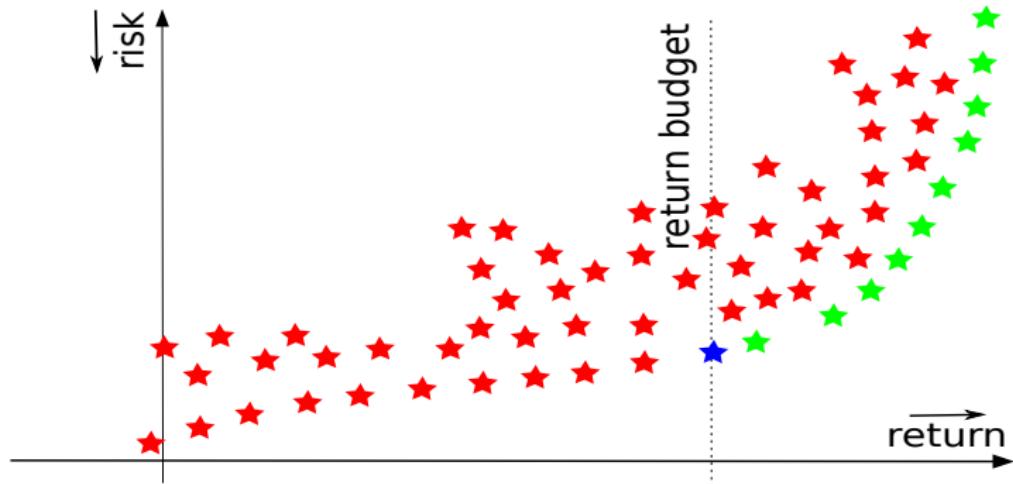
- ▶ \mathbb{R}^k with $k > 1$ has no total order \implies no “best” solution, only non-dominated ones on the Pareto frontier
- ▶ Two practical solutions:



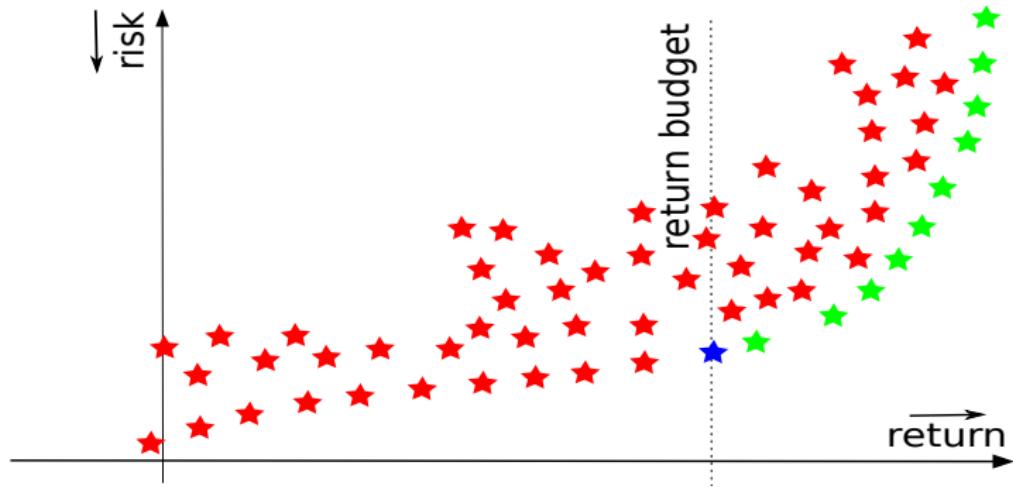
- ▶ \mathbb{R}^k with $k > 1$ has no total order \Rightarrow no “best” solution, only non-dominated ones on the Pareto frontier
- ▶ Two practical solutions: maximize risk-adjusted return,
a.k.a. scalarization $\min \{ f_1(x) + \alpha f_2(x) : x \in X \}$ (which $\alpha??$)



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- ▶ Two practical solutions: maximize return with budget on maximum risk, a.k.a. budgeting $\min \{ f_1(x) : f_2(x) \leq \beta_2, x \in X \}$ (which β_2 ??)



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a.k.a. budgeting $\min \{ f_2(x) : f_1(x) \geq \beta_1, x \in X \}$ (which β_1 ??)
- ▶ All a bit fuzzy, but it's the nature of the beast
- ▶ We always assume this done if necessary at modelling stage
(regularization, grid search used to divine hyperparameters α, β_1, β_2)

- (Euclidean) scalar product of $x \in \mathbb{R}^n$ and $z \in \mathbb{R}^n$:

$$\langle x, z \rangle = \sum_{i=1}^n x_i z_i = x_1 z_1 + \cdots + x_n z_n$$

- (Euclidean) norm: $\|x\| := \sqrt{x_1^2 + \cdots + x_n^2} = \sqrt{\langle x, x \rangle}$ (induced by $\langle \cdot, \cdot \rangle$)

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$$\theta = 0$$

► Geometric interpretation: $\langle x, z \rangle = \|x\| \cdot \|z\| \cdot \cos(\theta)$

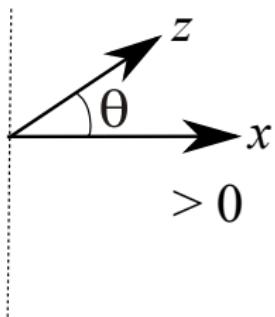

$$z \quad x$$

$\langle x, z \rangle > 0 \equiv$ "x and z point in the same direction"

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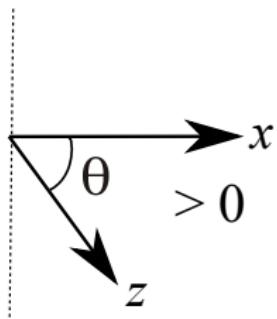


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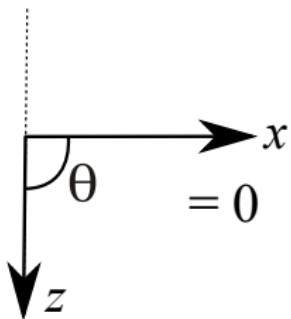


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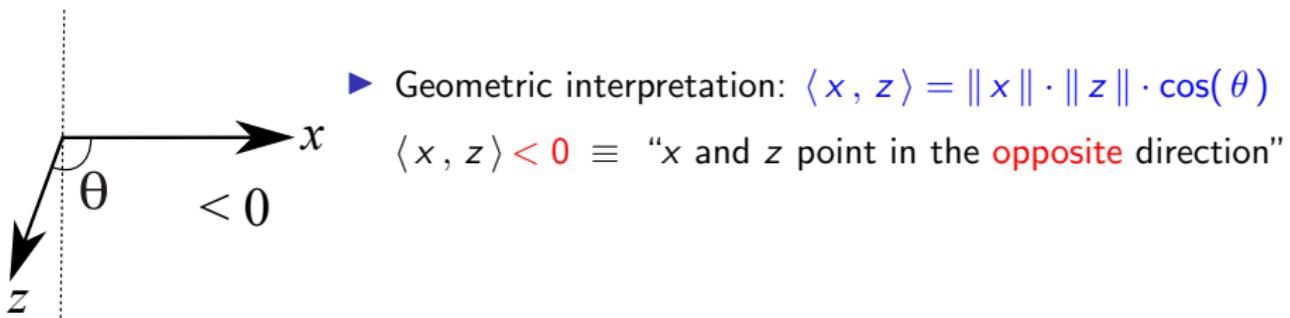
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$$\langle x, z \rangle = 0 \equiv x \perp z \text{ (orthogonal)}$$

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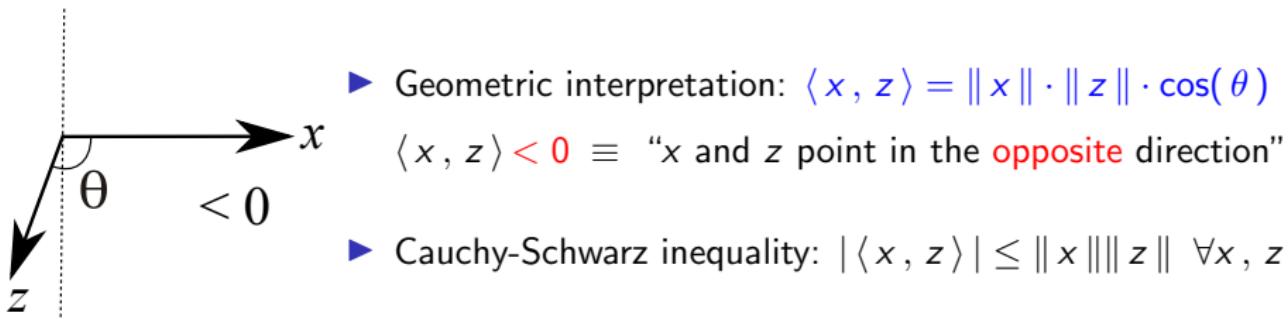
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- (Euclidean) distance between x and z = norm of x when z is the origin:

$$d(x, z) := \|x - z\| = \sqrt{(x_1 - z_1)^2 + \cdots + (x_n - z_n)^2}$$

- Ball, center $x \in \mathbb{R}^n$, radius $r > 0$: $\mathcal{B}(x, r) = \{z \in \mathbb{R}^n : \|z - x\| \leq r\}$

- $\mathbb{R}^n \in$ vector space \equiv closed under sum and scalar multiplication

$$x + z = [x_1 + z_1, \dots, x_n + z_n], \quad \alpha x = [\alpha x_1, \dots, \alpha x_n]$$

- Finite-dimensional vector space: $\{u^i\}_{i=1}^n$ finite base s.t. $\forall x \in \mathbb{R}^n \exists \alpha_1, \dots, \alpha_n$ s.t. $x = \alpha_1 u^1 + \dots + \alpha_n u^n$ (canonical base: $u_i^i = 1$, $u_h^i = 0$ for $h \neq i$, $\alpha_i = x_i$)
- Not all vector spaces are finite-dimensional (function spaces, ...)
- Properties \equiv definition of scalar product:
 1. $\langle x, z \rangle = \langle z, x \rangle \quad \forall x, z \in \mathbb{R}^n$ (symmetry)
 2. $\langle x, x \rangle \geq 0 \quad \forall x \in \mathbb{R}^n, \quad \langle x, x \rangle = 0 \iff x = 0$
 3. $\langle \alpha x, z \rangle = \alpha \langle x, z \rangle \quad \forall x \in \mathbb{R}^n, \alpha \in \mathbb{R}$
 4. $\langle x + w, z \rangle = \langle x, z \rangle + \langle w, z \rangle \quad \forall x, w, z \in \mathbb{R}^n$
- \exists other scalar products that make sense in other spaces
(matrices, integrable functions, random variables, ...)
- Not just theoretical stuff (cf. kernel in SVM)

► Properties \equiv definition of norm:

1. $\|x\| \geq 0 \quad \forall x \in \mathbb{R}^n, \quad \|x\| = 0 \iff x = 0$
2. $\|\alpha x\| = |\alpha| \|x\| \quad \forall x \in \mathbb{R}^n, \alpha \in \mathbb{R}$
3. $\|x + z\| \leq \|x\| + \|z\| \quad \forall x, z \in \mathbb{R}^n$ (triangle inequality)

► $\|x + z\|^2 = \|x\|^2 + \|z\|^2 + 2\langle x, z \rangle$ (only Euclidean norm)► $2\|x\|^2 + 2\|z\|^2 = \|x + z\|^2 + \|x - z\|^2$ (Parallelogram Law)► Properties \equiv definition of distance:

1. $d(x, z) \geq 0 \quad \forall x, z \in \mathbb{R}^n, \quad d(x, z) = 0 \iff x = z$
2. $d(\alpha x, 0) = |\alpha| d(x, 0) \quad \forall x \in \mathbb{R}^n, \alpha \in \mathbb{R}$
3. $d(x, w) \leq d(x, z) + d(z, w) \quad \forall x, w, z \in \mathbb{R}^n$ (triangle inequality)

► $\|\cdot\|$ defines $\mathcal{B}(\cdot, \cdot)$ \equiv the topology of the vector space:
what is next to what (will be useful later on)

- ▶ $\text{gr}(f) \in \mathbb{R}^{n+1}$, impossible if $n > 3$ ($n = 3$ hard already)
- ▶ $L(f, \cdot) \in \mathbb{R}^n$, impossible if $n > 4$ ($n = 4$ hard already)

- ▶ $\text{gr}(f) \in \mathbb{R}^{n+1}$, impossible if $n > 3$ ($n = 3$ hard already)
- ▶ $L(f, \cdot) \in \mathbb{R}^n$, impossible if $n > 4$ ($n = 4$ hard already)
- ▶ General $n, f : \mathbb{R}^n \rightarrow \mathbb{R}, x \in \mathbb{R}^n$ (origin), $d \in \mathbb{R}^n$ (direction):
 $\varphi_{x,d}(\alpha) = f(x + \alpha d) : \mathbb{R} \rightarrow \mathbb{R}$ tomography of f from x along d
- ▶ $\text{gr}(\varphi_{x,d})$ can always be pictured, but too many of them: which x, d ?
- ▶ $\|d\|$ only changes the scale: $\varphi_{x,\beta d}(\alpha) = \varphi_{x,d}(\beta \alpha)$ (check) \implies often (but not always) convenient to use normalised direction ($\|d\| = 1$)
- ▶ Simplest case: restriction along i -th coordinate ($\|u^i\| = 1$)
 $f_x^i(\alpha) = f(x_1, \dots, x_{i-1}, \alpha, x_{i+1}, \dots, x_n) \equiv \varphi_{[x_1, \dots, x_{i-1}, 0, x_{i+1}, \dots, x_n], u^i}(\alpha)$
- ▶ For small n can “look at all d ”
- ▶ Otherwise, find the specific d that “shows what you want to see”
- ▶ When x and d clear from context (will happen a lot), just $\varphi(\alpha)$

- Linear function: $f(x) = \langle b, x \rangle = \sum_{i=1}^n b_i x_i$, **fixed** $b \in \mathbb{R}^n$
- Linear \equiv i. $f(\gamma x) = \gamma f(x)$, ii. $f(x+z) = f(x) + f(z) \quad \forall x, \gamma, z$

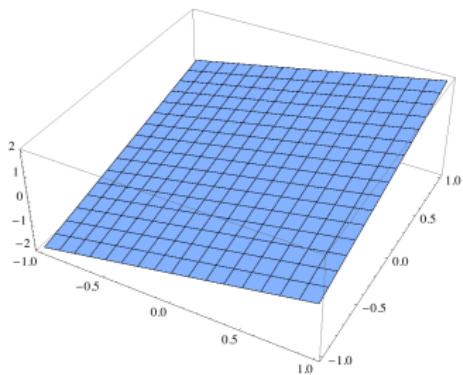
Exercise: Linear \implies i) + ii) trivial, prove \Leftarrow ; extends to **affine** ($\dots + c$)?

- $\langle b, x \rangle = \sum_{i=1}^n [f_i(x_i) = b_i x_i]$, **sum of n univariate linear functions**

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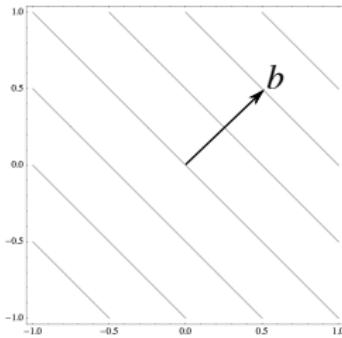
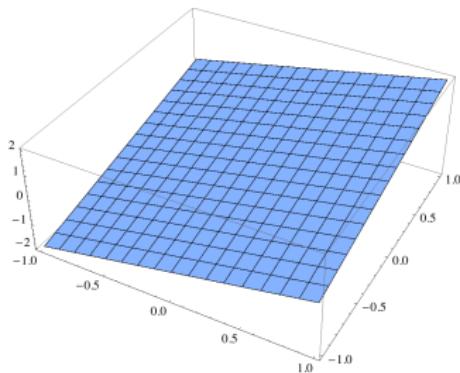


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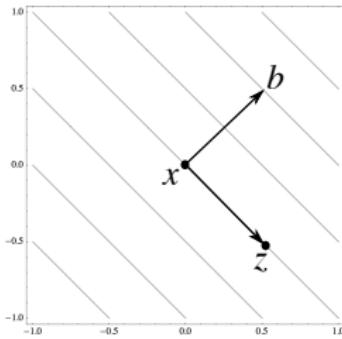
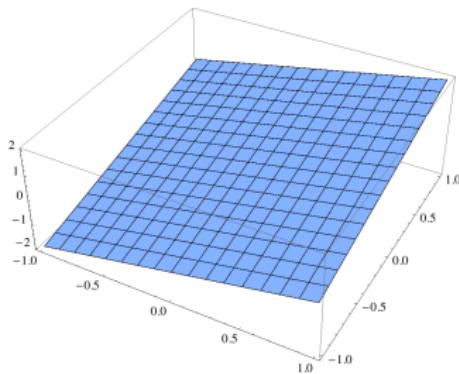


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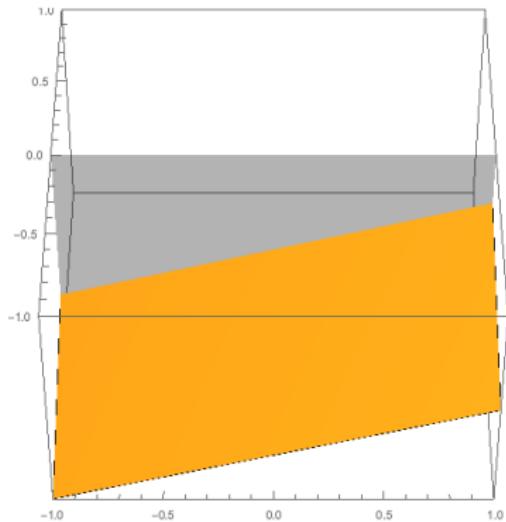
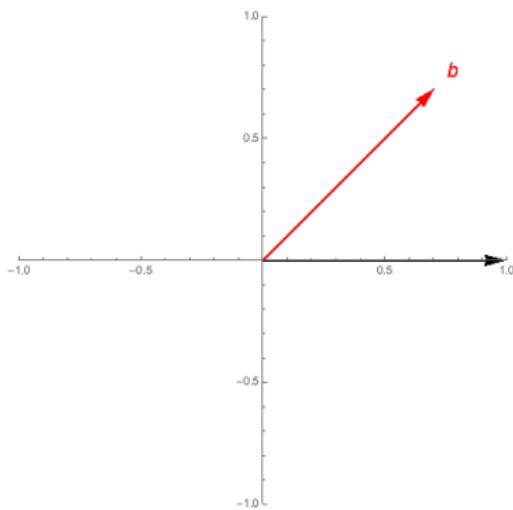
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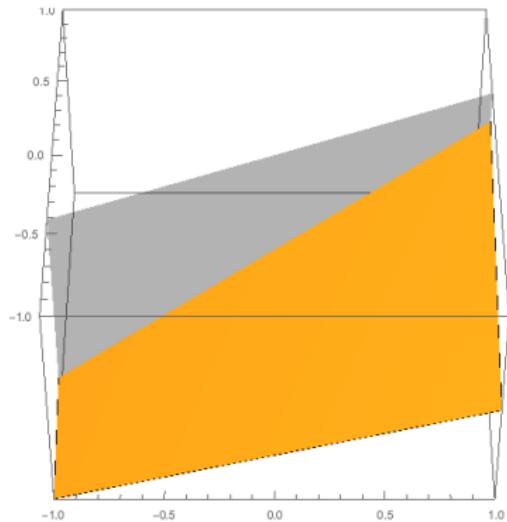
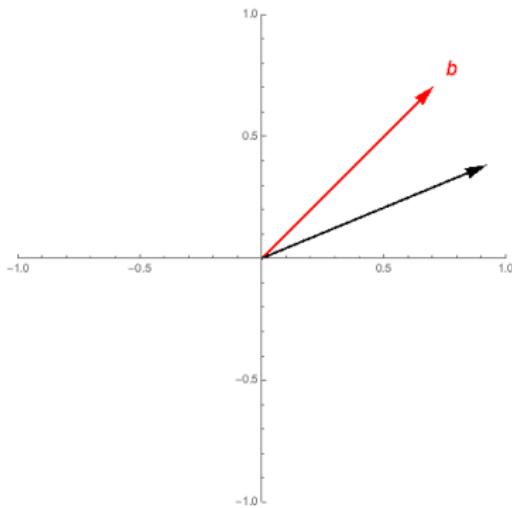
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 $f(x) = f(z) \equiv \langle b, x \rangle = \langle b, z \rangle \equiv \langle b, z - x \rangle = 0 \equiv b \perp z - x$

- $f(x) = \langle b, x \rangle$, $x = 0$, $\|d\| = 1$: $\varphi(\alpha) = \alpha \langle b, d \rangle = \alpha \|b\| \cos(\theta)$

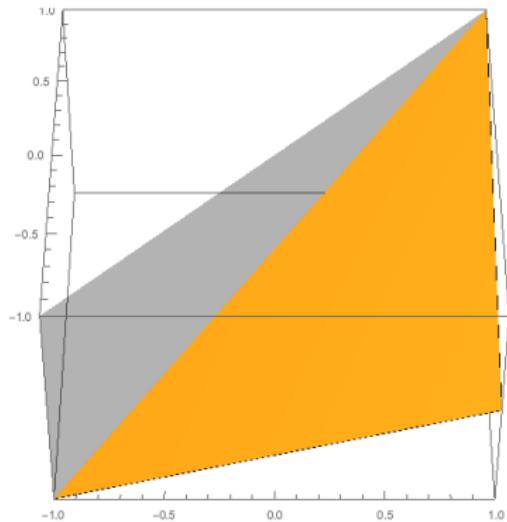
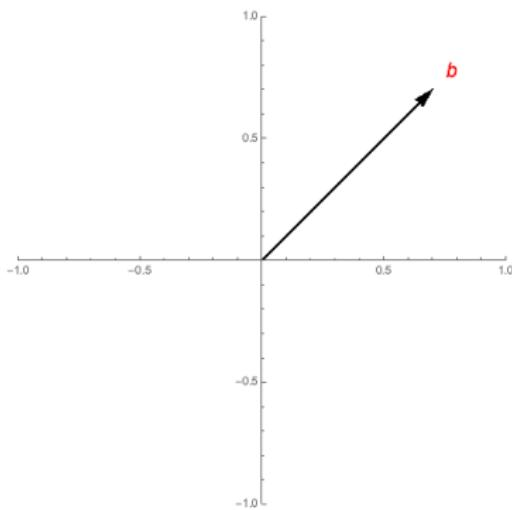
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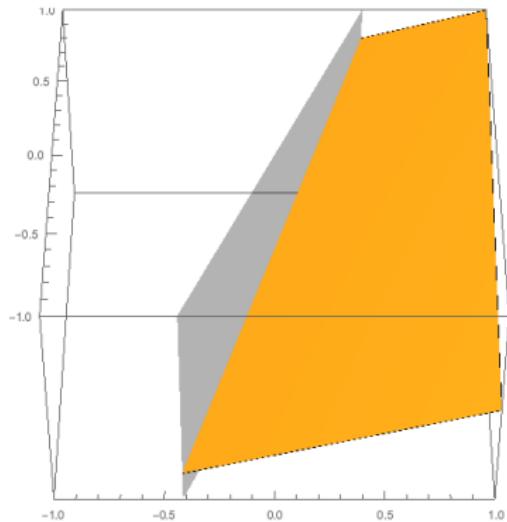
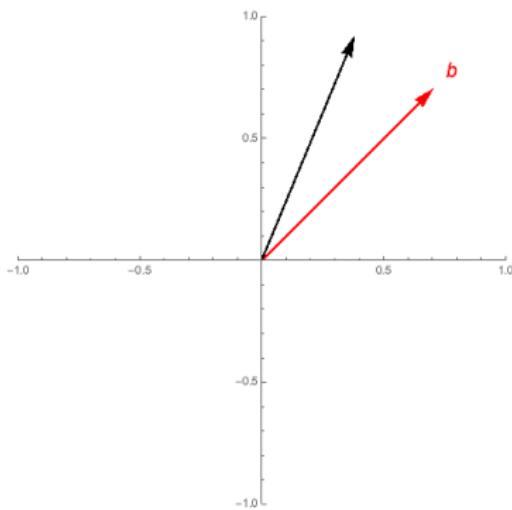
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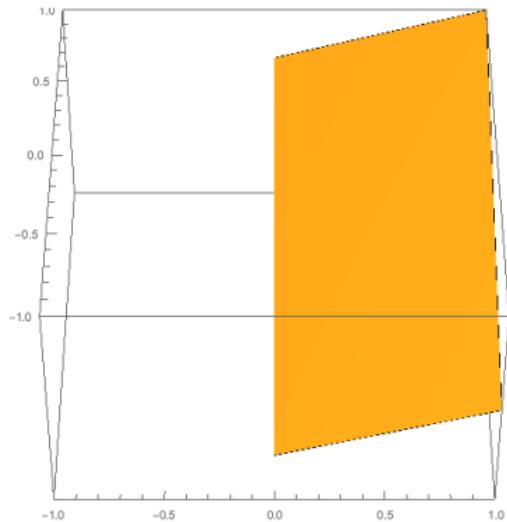
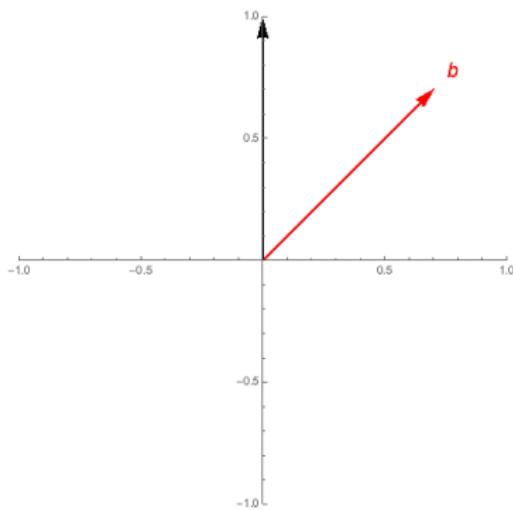
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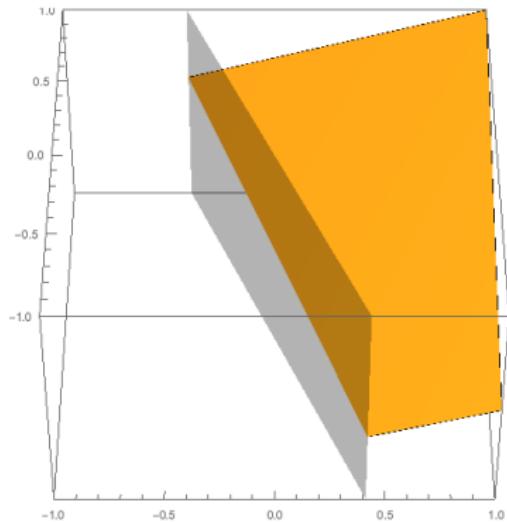
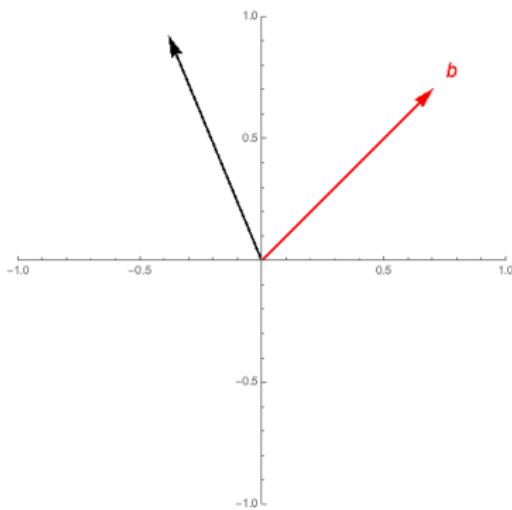
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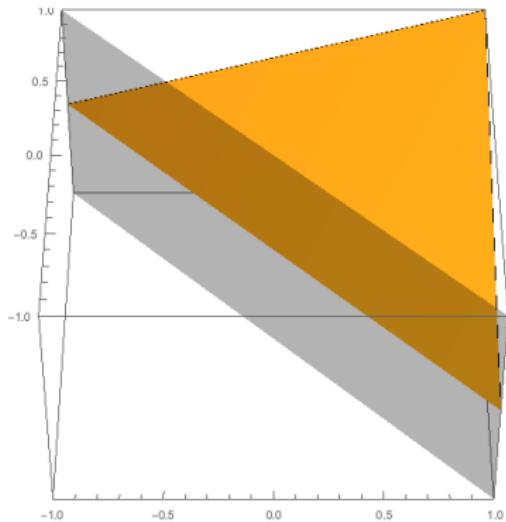
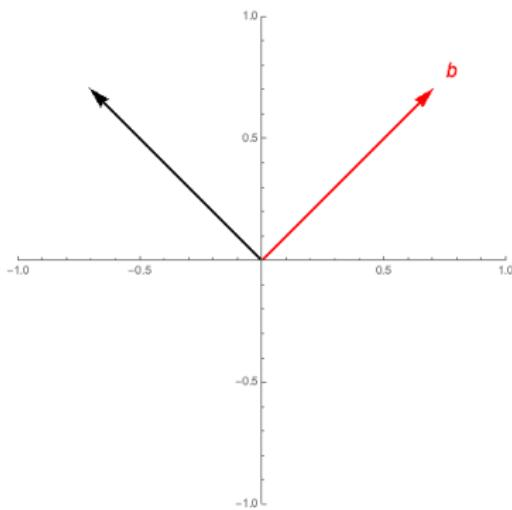
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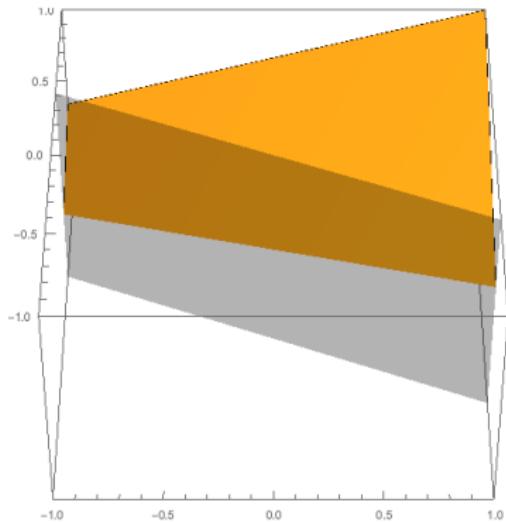
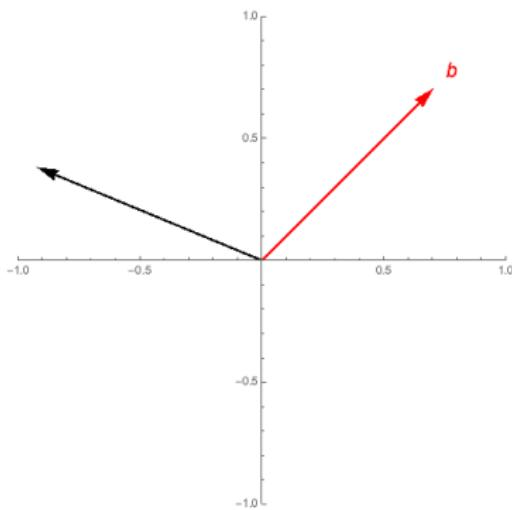
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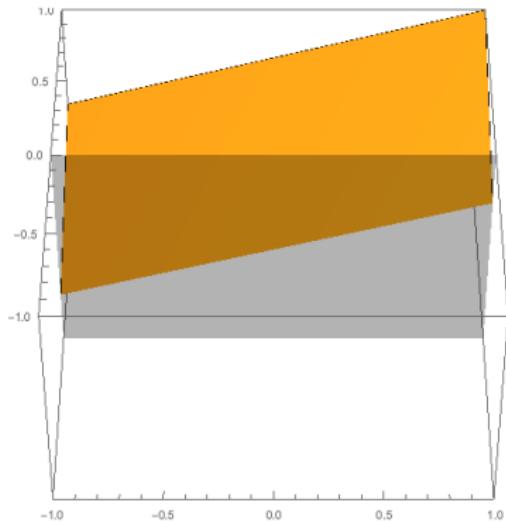
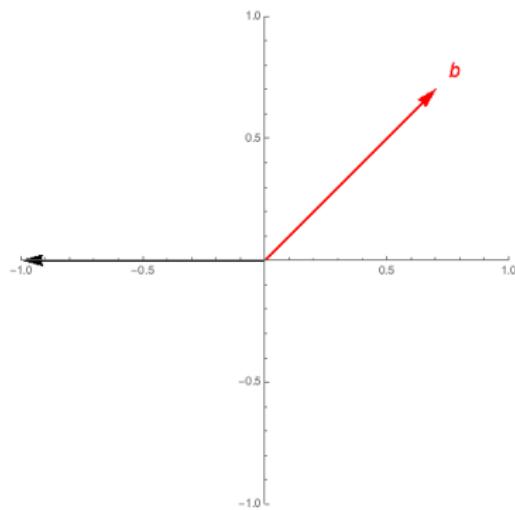
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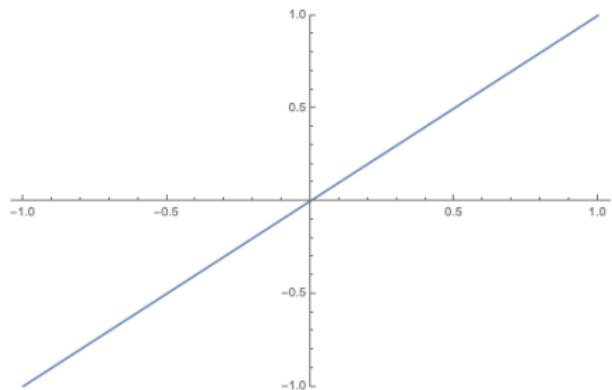
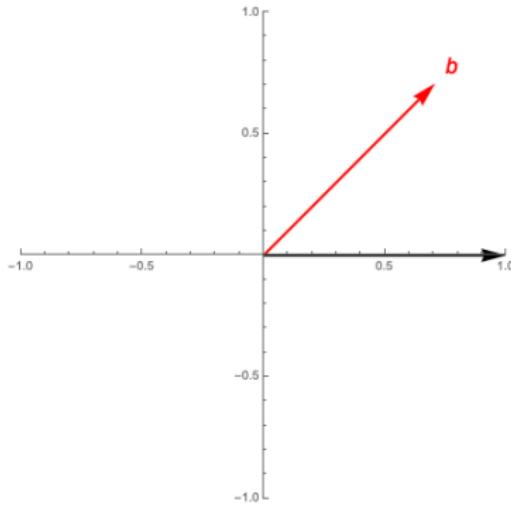
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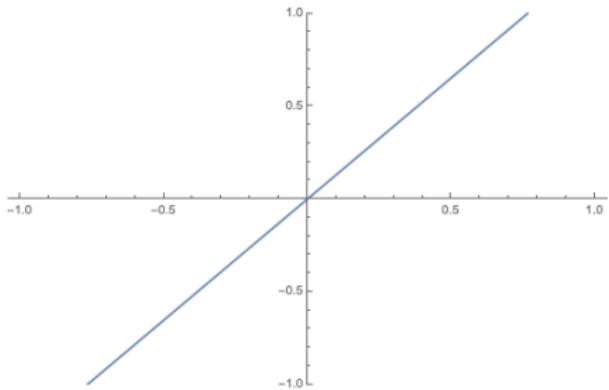
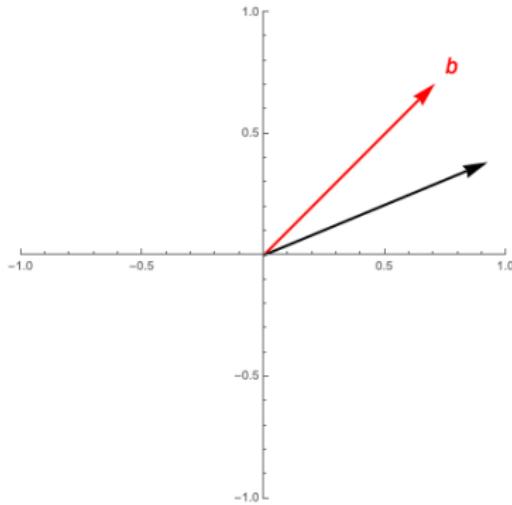


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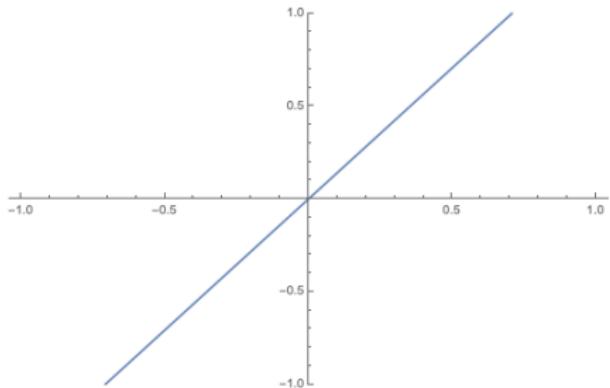
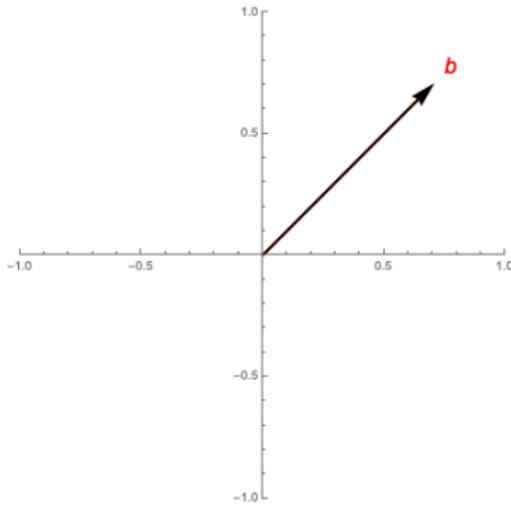
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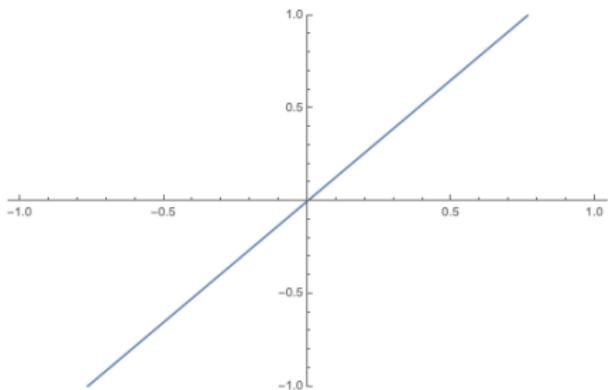
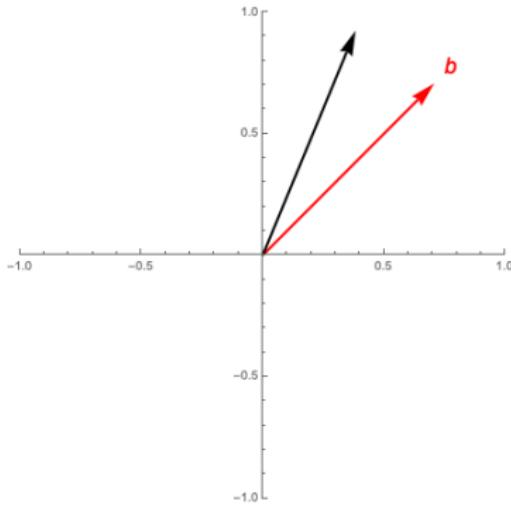
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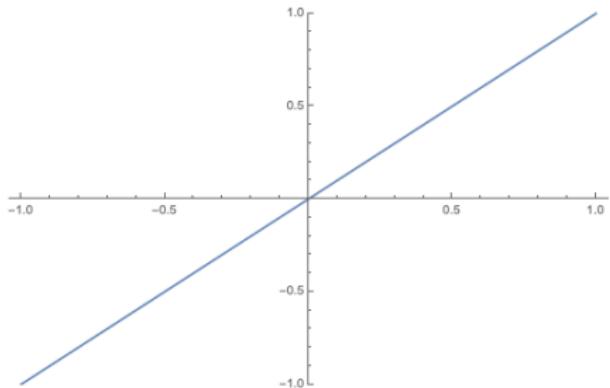
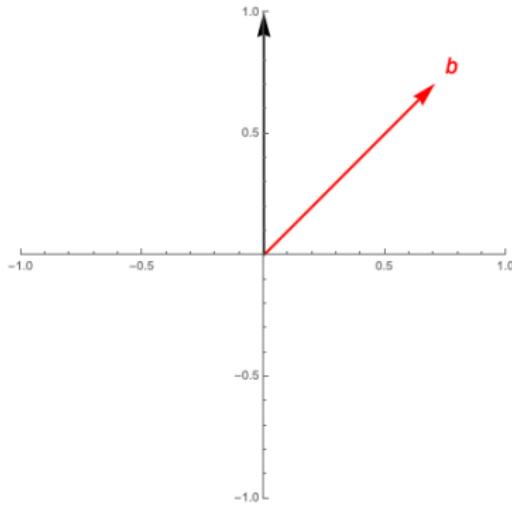
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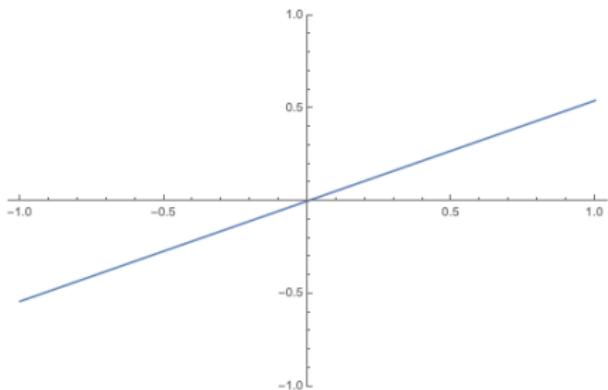
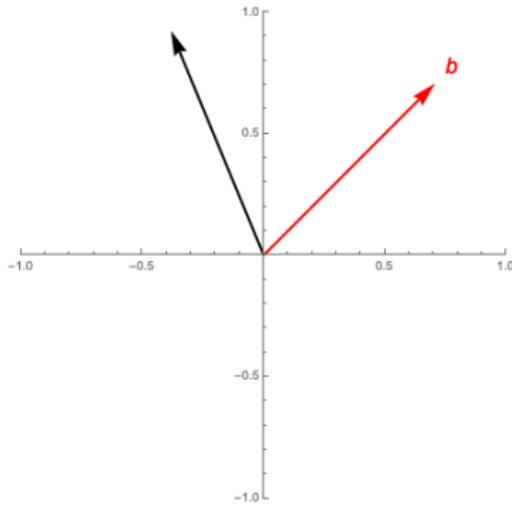
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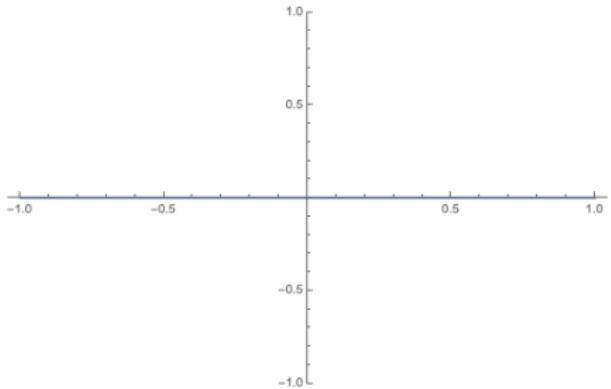
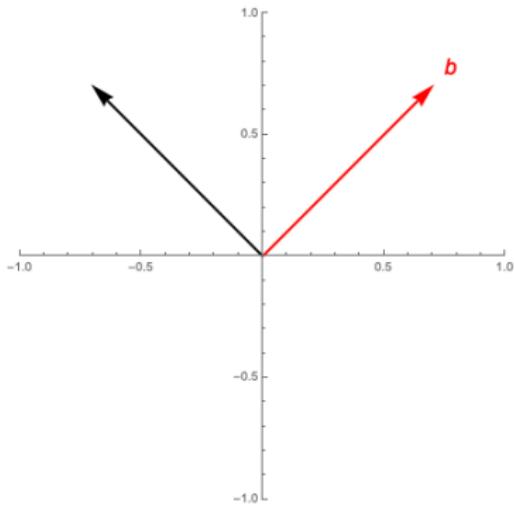
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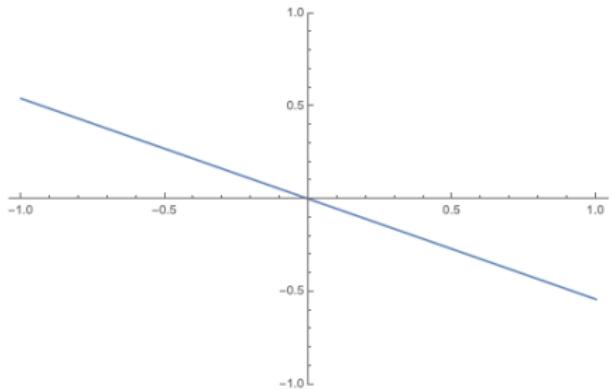
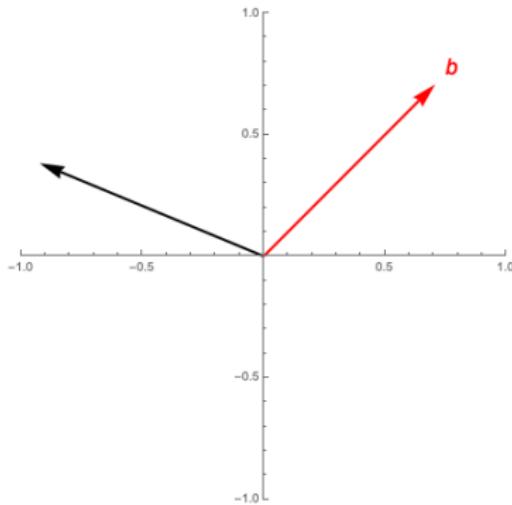
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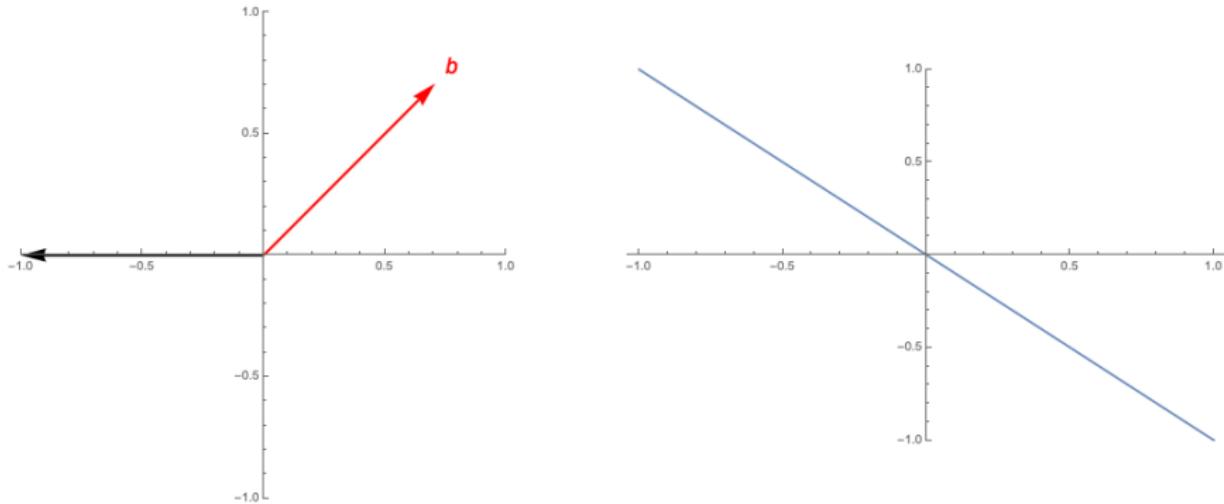
- “Flat” if $d \perp b$

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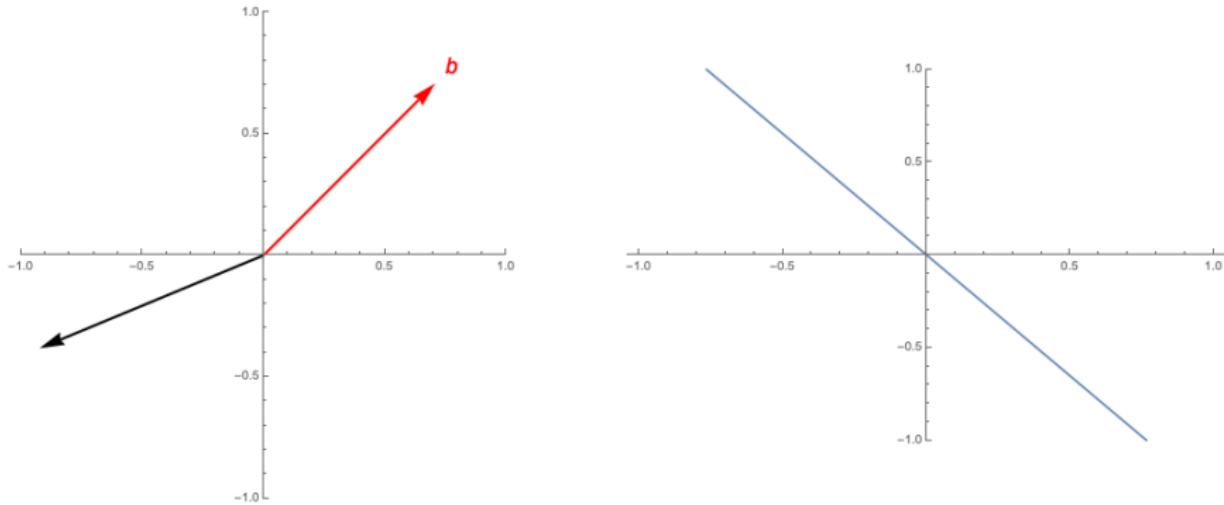
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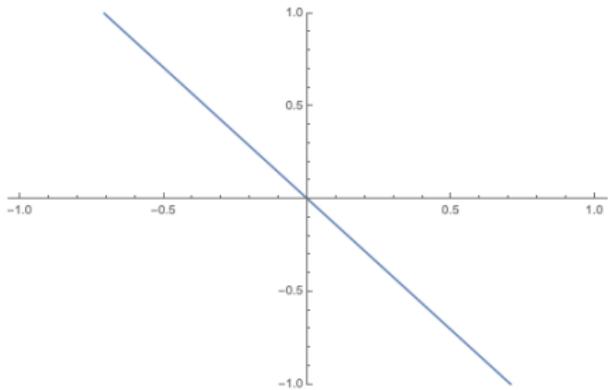
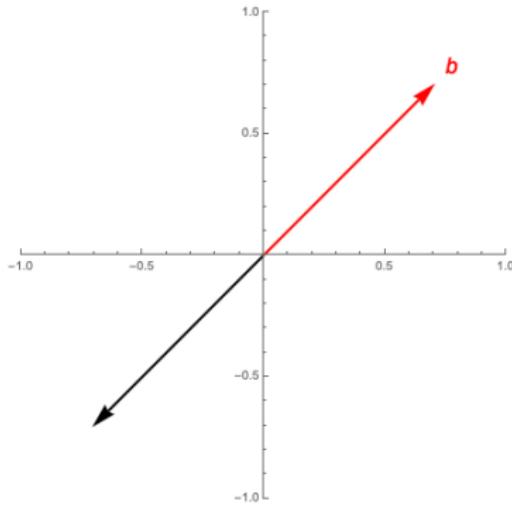
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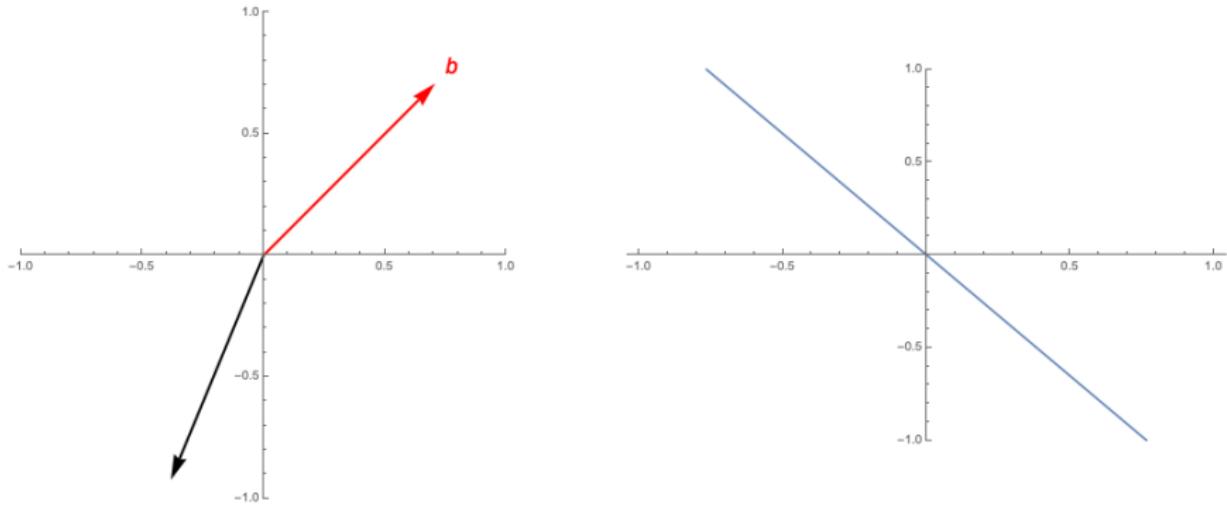
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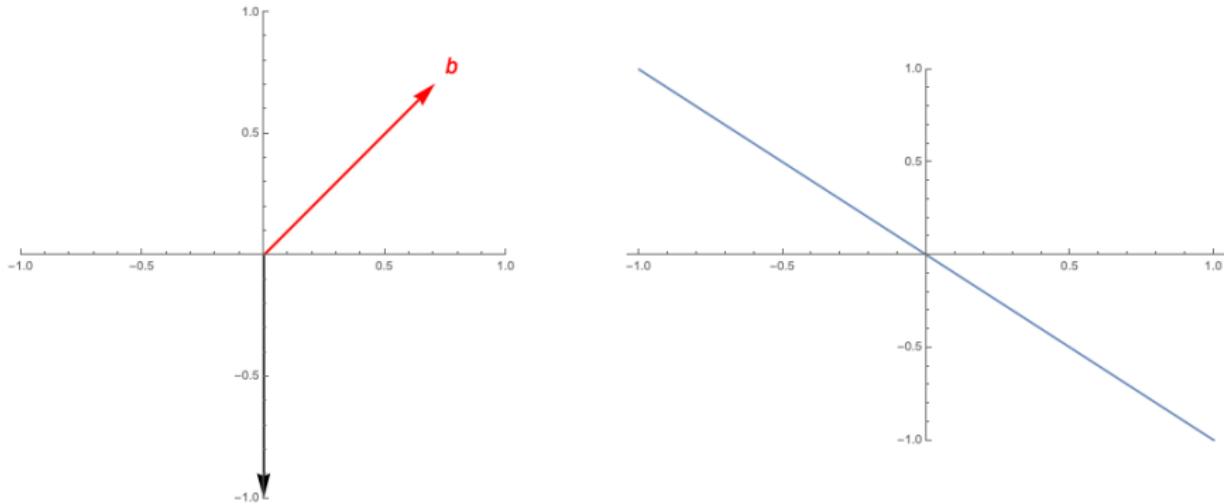
- Decreasing if “ b opposite direction as d ”, collinear \implies steepest (negative)

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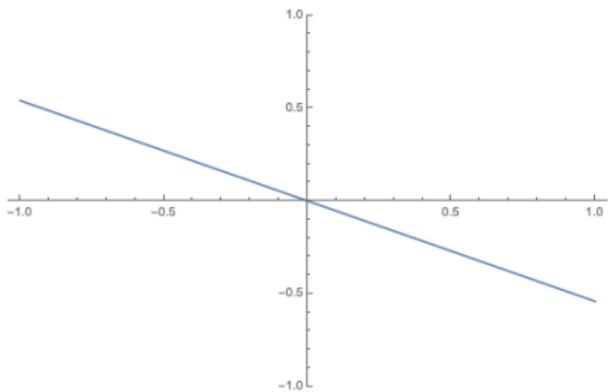
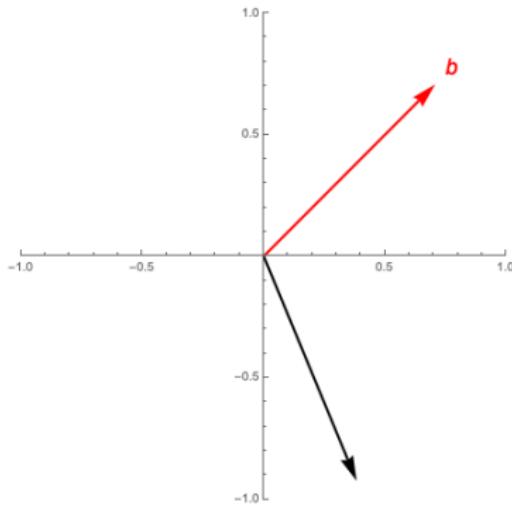
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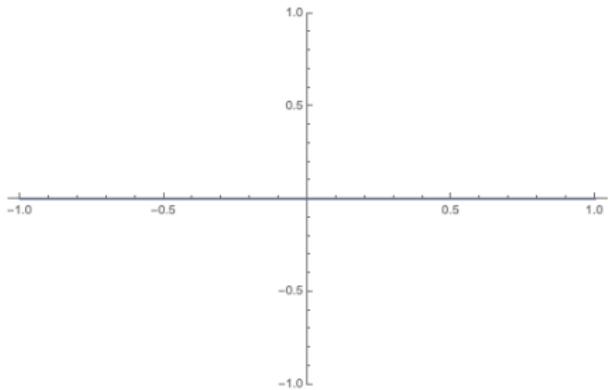
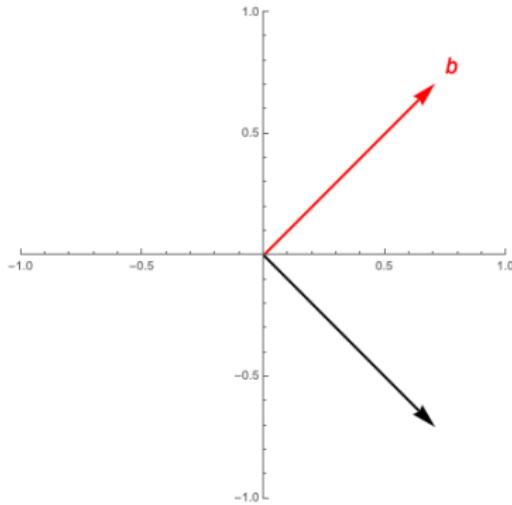
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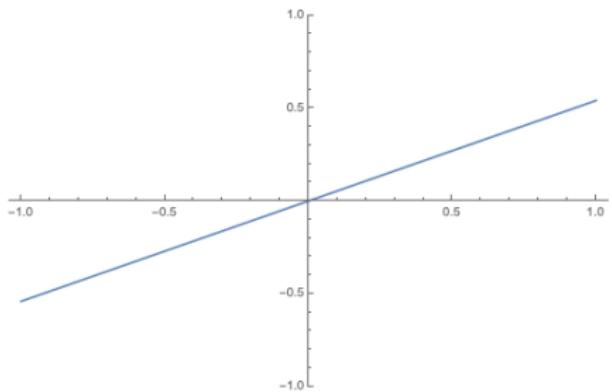
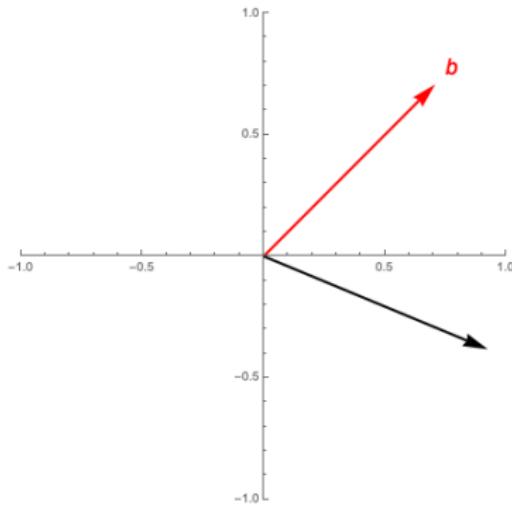
- Decreasing if “ b opposite direction as d ”, “less collinear” \implies less steep

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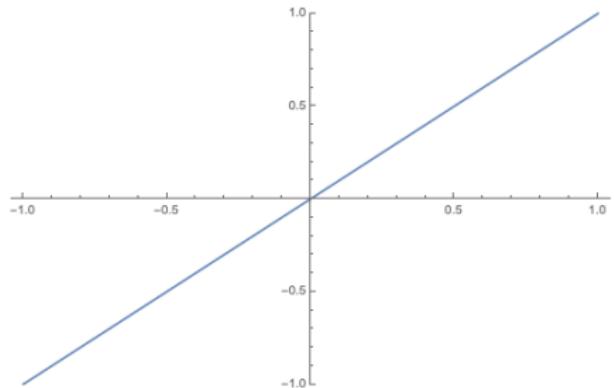
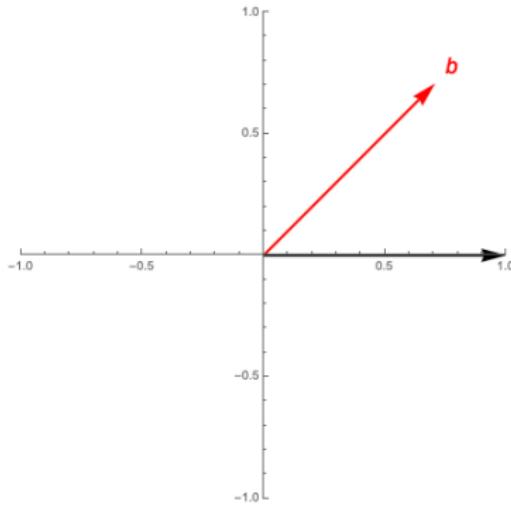
- “Flat” if $d \perp b$

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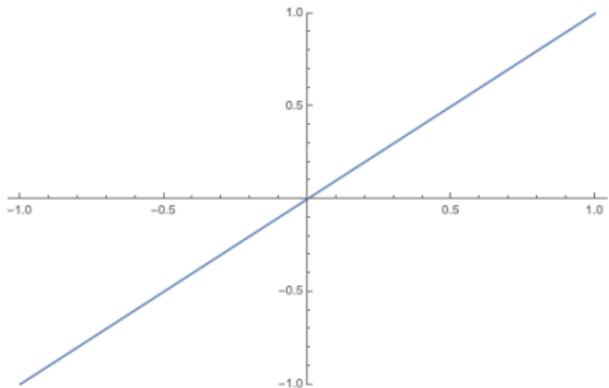
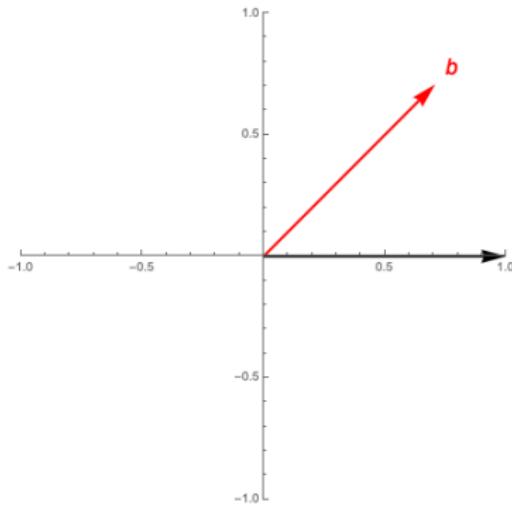
- Increasing if “ b in the same direction as d ”

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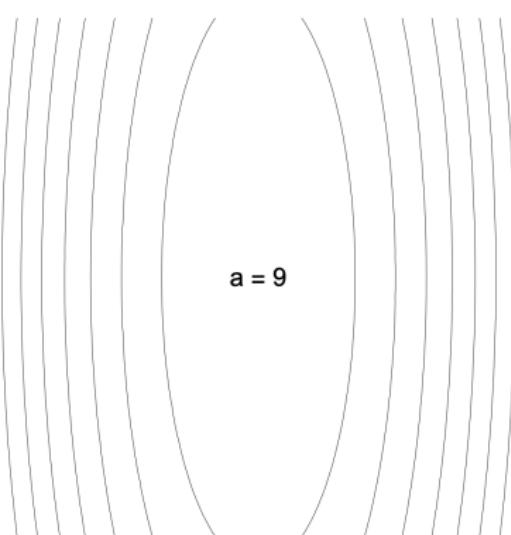
- Increasing if “ b in the same direction as d ”
- $f_* = \min\{f(x)\} = -\infty$ except if $b = 0$, in which case $f_* = 0$ (same for max)
- $\min\{f(x) : x \in X\}$, X hyperrectangle, ► Optimizing a linear function (same for max)
n independent problems, as nothing links x_i and x_j for $i \neq j$
- *n* closed formulæ $O(1)$ each, almost the last time

- Separable (non-homogeneous) quadratic function:

$$f(x) = \sum_{i=1}^n [f_i(x_i) = a_i x_i^2 + b_i x_i], \text{ fixed } (a, b) \in \mathbb{R}^{2n}$$

= sum of n univariate quadratic (non-homogeneous) functions

- $f(x) = \|x\|^2 = \sum_{i=1}^n x_i^2$ an important special case



- $f(x_1, x_2) = ax_1^2 + x_2^2 [+0x_1 + 0x_2]$
- Contour plots for different values of a

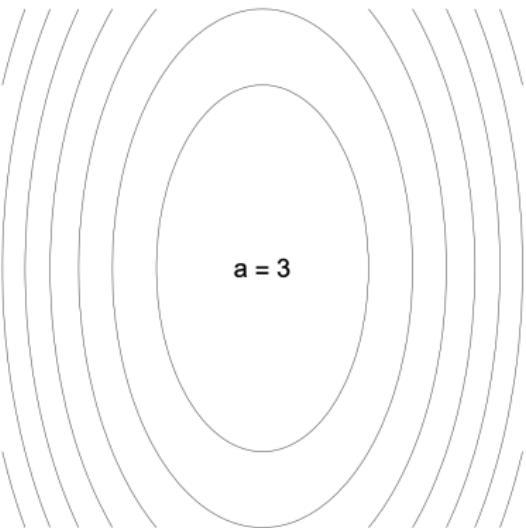
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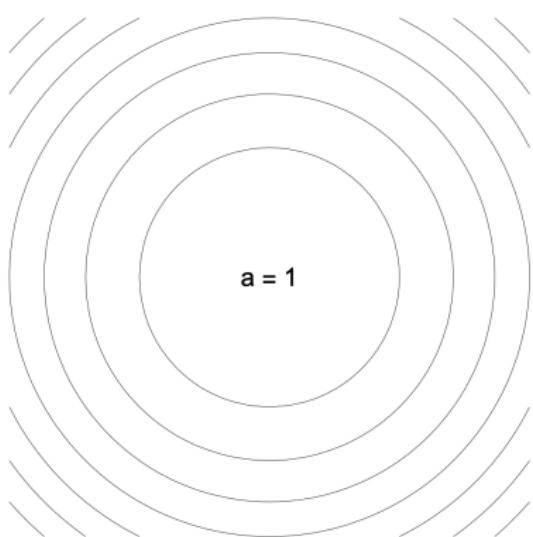
$a = 3$

- Separable (non-homogeneous) quadratic function:

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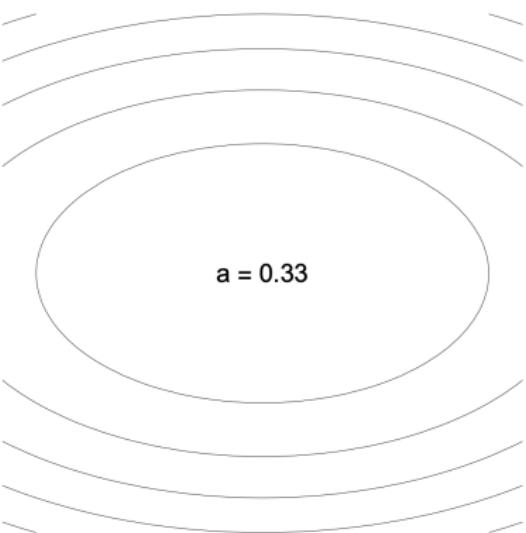
- $f(x_1, x_2) = ax_1^2 + x_2^2 [+0x_1 + 0x_2]$
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- For $a = 1$, perfect circles

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a = 0.33

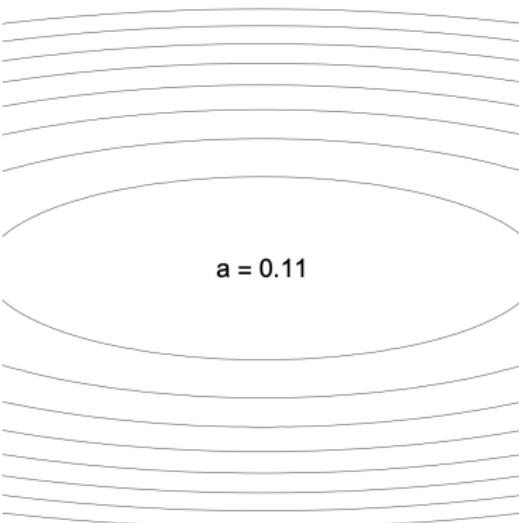
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- For $a = 1$, perfect circles
- Larger / smaller a , more \uparrow / \leftrightarrow elongated

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a = 0.11

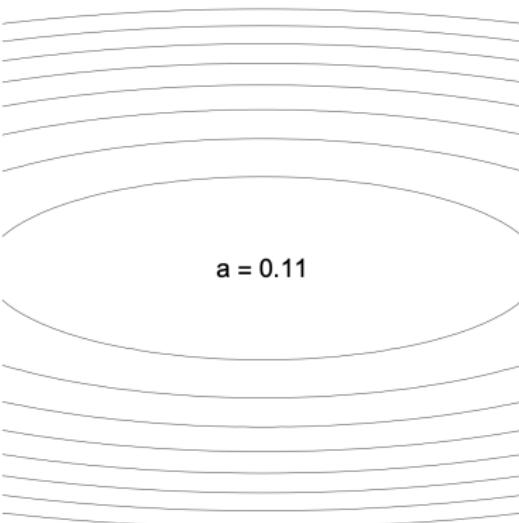
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- Could be non-homogeneous,
 $[0, 0] \rightarrow [-b_1/2a_1, -b_2/2a_2]$
- $O(n)$ ► Optimizing a quadratic non-homogeneous function ,
this is the last time

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- $O(n)$ ► Optimizing a quadratic non-homogeneous function ,
this is the last time
- Not a general quadratic function, coming right next

- Nonseparable homogeneous quadratic function: fixed $Q \in \mathbb{R}^{n \times n}$ (n $Q_i \in \mathbb{R}^n$)

$$f(x) = \frac{1}{2}x^T Qx = \frac{1}{2} \left[\sum_{i=1}^n Q_{ii} x_i^2 + \sum_{i=1}^n \sum_{j=1, j \neq i}^n Q_{ij} x_i x_j \right]$$

- Not linear: $f(x+z) = \frac{1}{2}(x+z)^T Q(x+z) = f(x) + f(z) + z^T Qx$

- W.l.o.g. Q symmetric:

$$x^T Qx = [(x^T Qx) + (x^T Qx)^T] / 2 = x^T [(Q + Q^T) / 2] x$$

- f symmetric: $f(x) = f(-x) \implies$ “centred in $x = 0$ ”

- Tomography: $\varphi(\alpha) = f(\alpha d) = \frac{1}{2}\alpha^2(d^T Qd) \implies$
homogeneous quadratic univariate, sign and steepness depend on $d^T Qd$

- Need to know about signs of $d^T Qd$ when d changes: (multi)linear algebra

- Crucial stuff: spectral decomposition, eigenvalues, eigenvectors of Q

- ▶ $Q \in \mathbb{R}^{n \times n}$, $v \in \mathbb{R}^n$, $\lambda \in \mathbb{R}$ s.t. $Qv = \lambda v$: v eigenvector of Q , λ eigenvalue
- ▶ v eigenvector $\equiv Qv = \lambda v \equiv Q(-v) = \lambda(-v) \equiv -v$ eigenvector
- ▶ Q symmetric \implies has n distinct eigenvectors H_1, H_2, \dots, H_n and n (not necessarily distinct) corresponding real eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$
- ▶ Eigenvectors can always be taken orthonormal: $H_i \perp H_j$ for $i \neq j$, $\|H_i\| = 1$ \implies linearly independent (check) \implies a(n orthonormal) basis of \mathbb{R}^n
- ▶ Spectral decomposition: $H = [H_1, \dots, H_n] \in \mathbb{R}^{n \times n}$, $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$

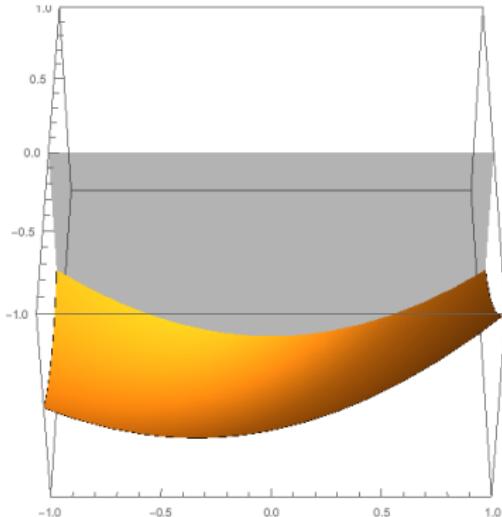
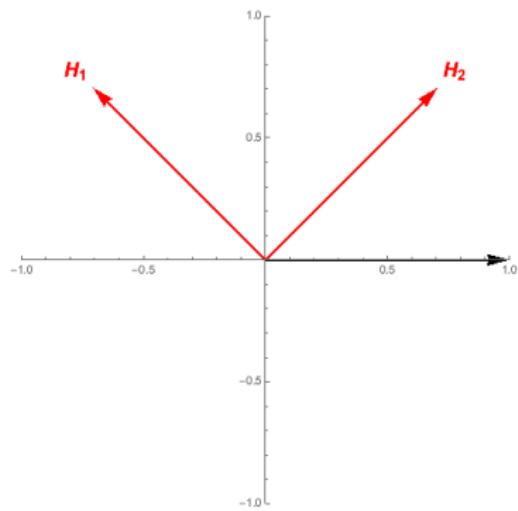
$$Q = H\Lambda H^T = \lambda_1 H_1 H_1^T + \dots + \lambda_n H_n H_n^T \quad (\text{check})$$
- ▶ Notation: $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ ($\lambda_1 = \max$, $\lambda_n = \min$)
- ▶ Variational characterization of eigenvalues:

$$\lambda_1 = \max\{d^T Q d / d^T d : d \neq 0\} = \max\{d^T Q d : \|d\| = 1\}$$

$$\lambda_n = \min\{d^T Q d / d^T d : d \neq 0\} = \min\{d^T Q d : \|d\| = 1\}$$
- ▶ $Q \succ 0$ = positive definite if $\lambda_i > 0 \forall i \equiv \lambda_n > 0 \equiv d^T Q d > 0 \forall d \neq 0$
 $Q \succeq 0$ = positive semi-definite if $\lambda_i \geq 0 \forall i \equiv \lambda_n \geq 0 \equiv d^T Q d \geq 0 \forall d \neq 0$
negative definite (\prec), semi-definite (\preceq), indefinite (\times) obvious

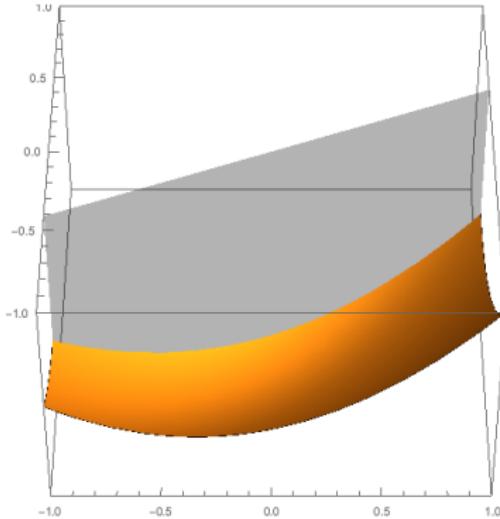
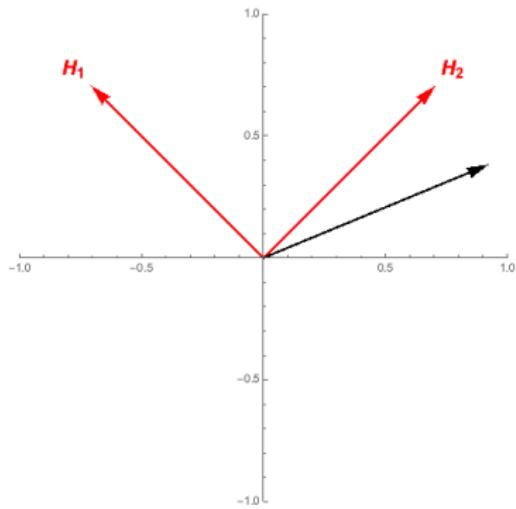
- Fundamental relation: $\varphi_{H_i}(\alpha) = \alpha^2 \lambda_i$ (check)

- $Q = \begin{bmatrix} 6 & -2 \\ -2 & 6 \end{bmatrix} \succ 0 \quad H = \frac{\sqrt{2}}{2} \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} \quad \lambda = \begin{bmatrix} 8 \\ 4 \end{bmatrix}$



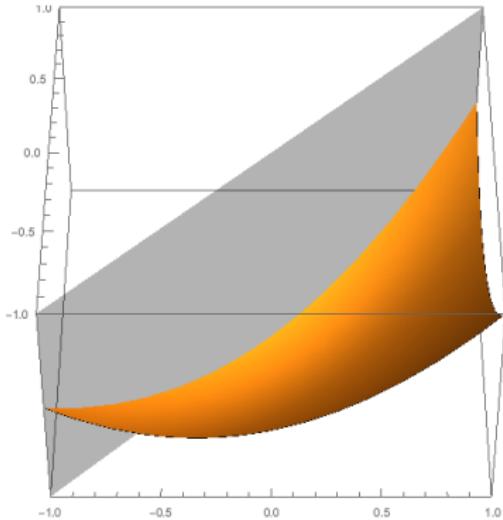
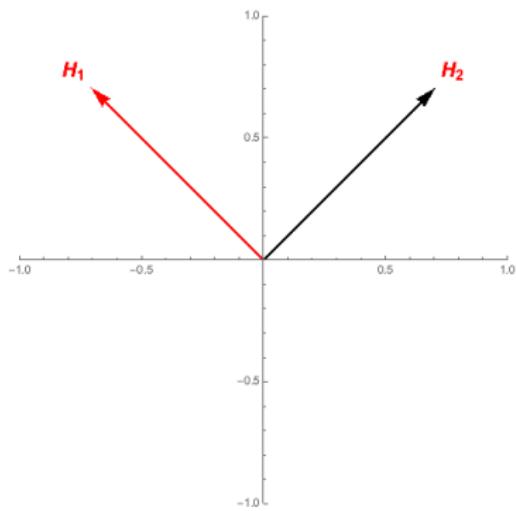
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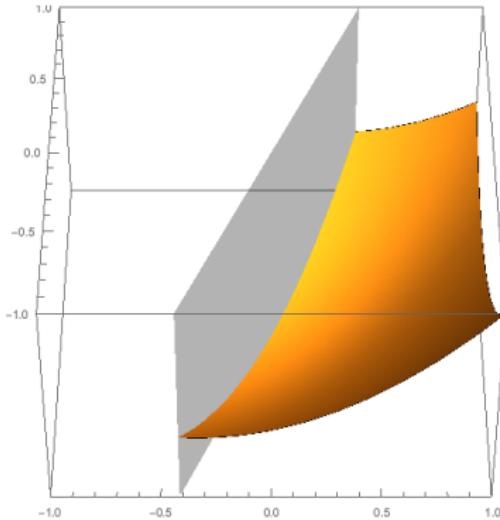
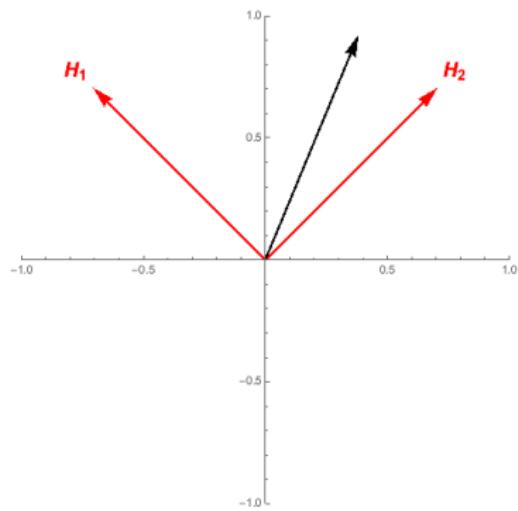
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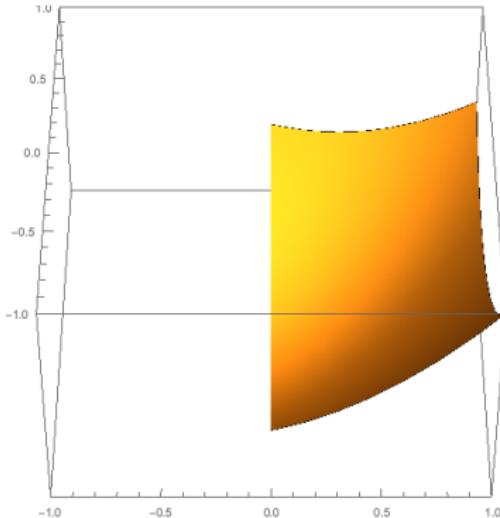
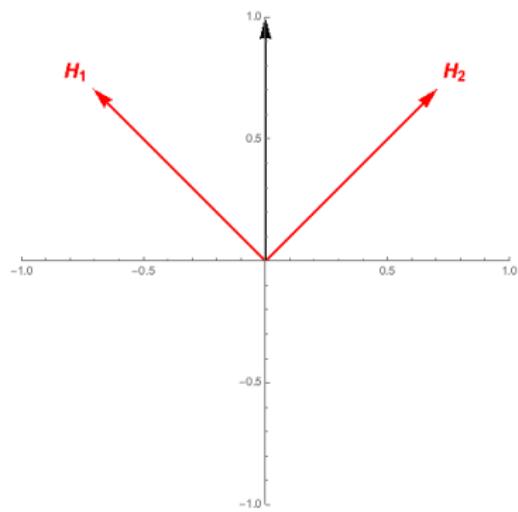
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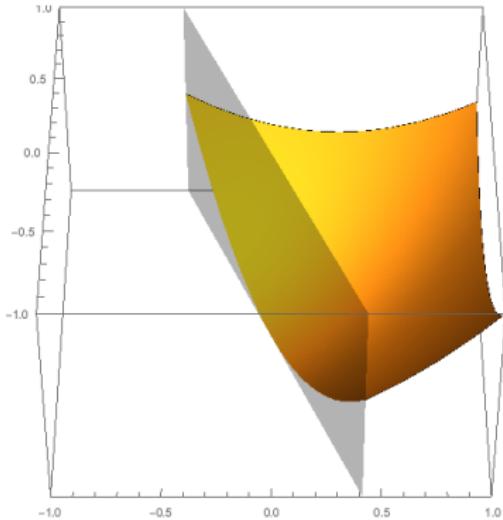
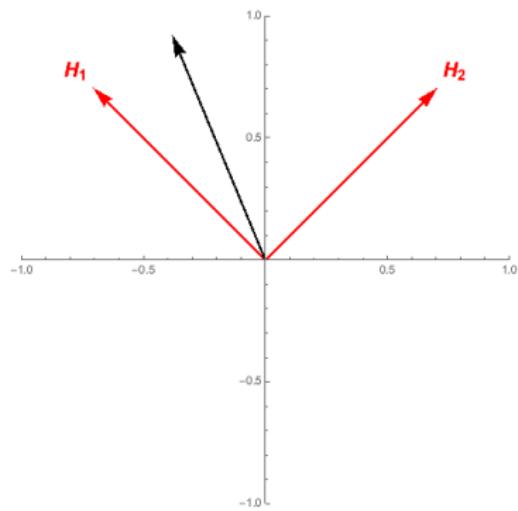
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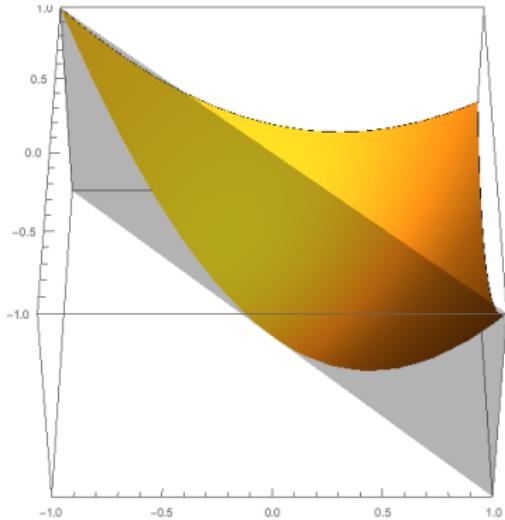
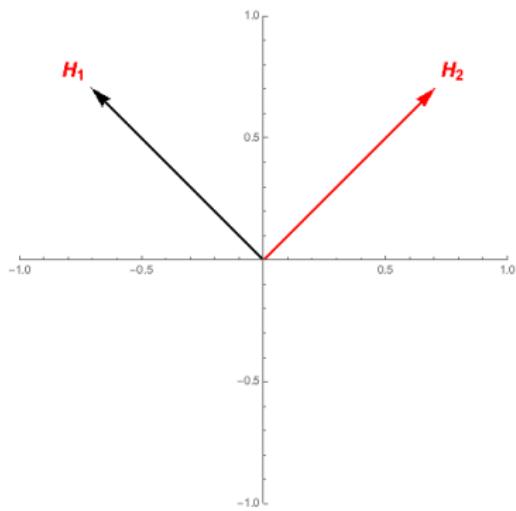
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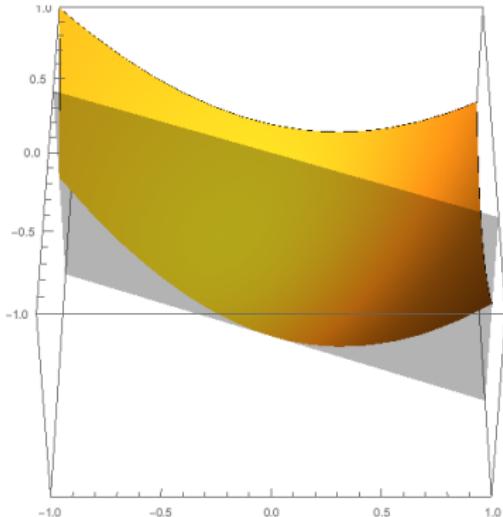
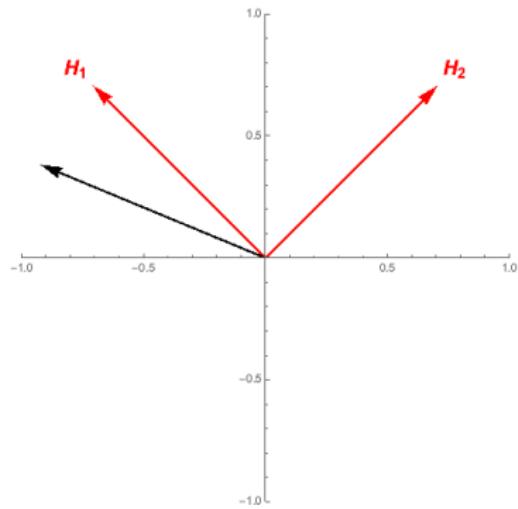
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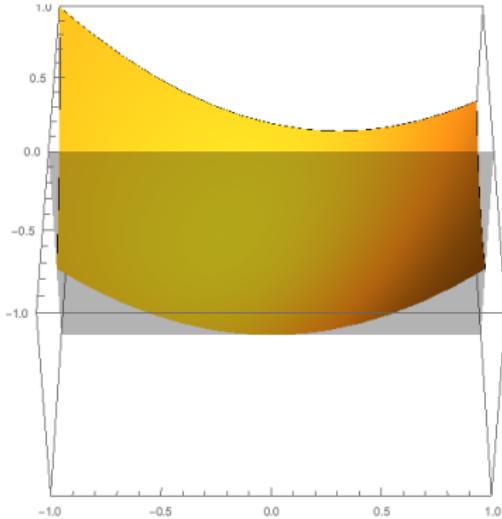
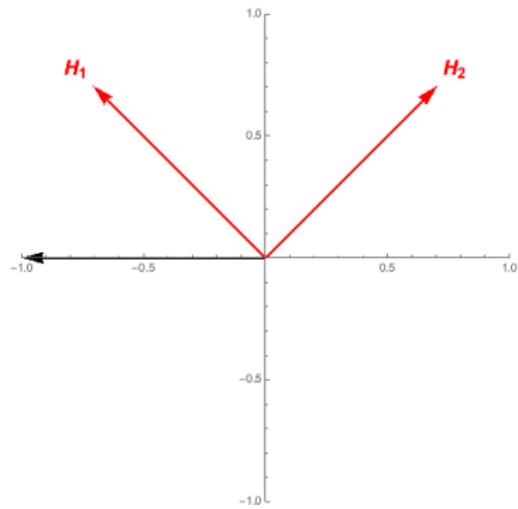
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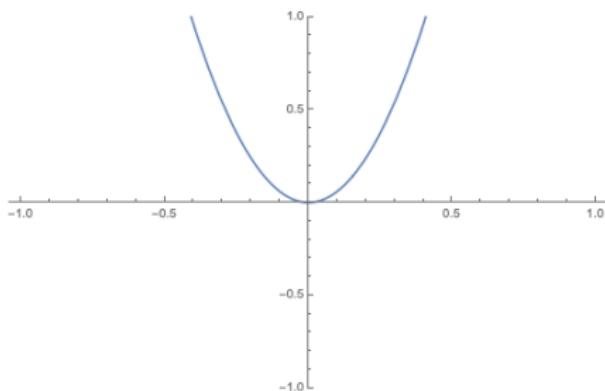
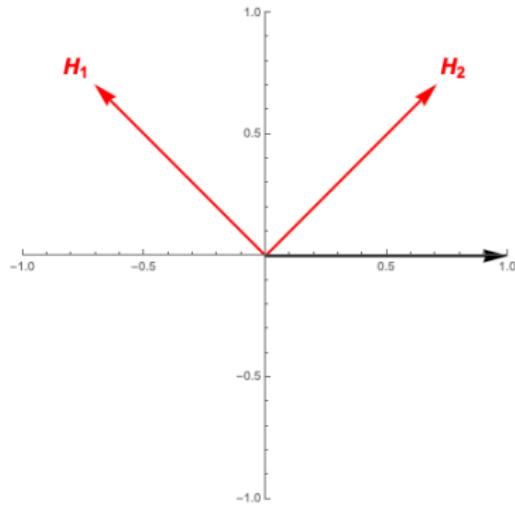
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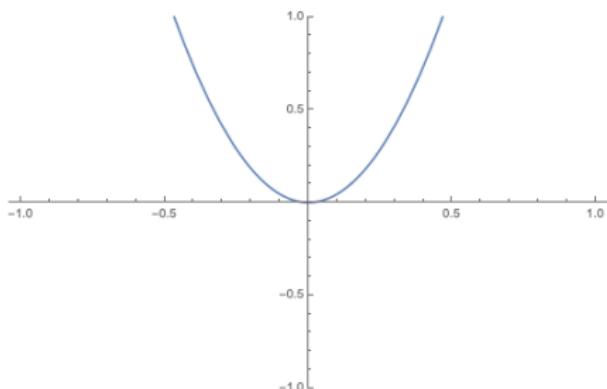
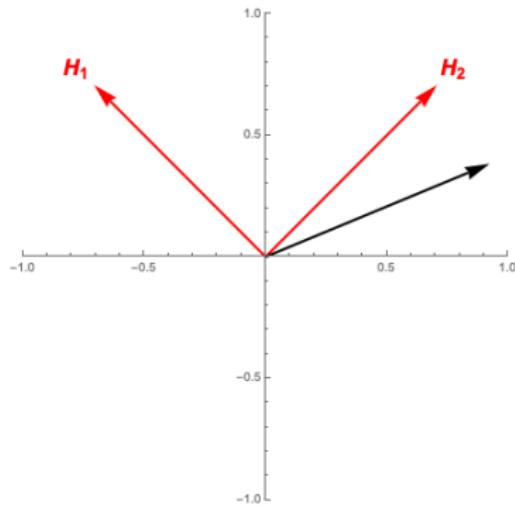


- $d^T Q d > 0 \forall d$, steepness change with d



- Fundamental relation: $\varphi_{H_i}(\alpha) = \alpha^2 \lambda_i$ (check)

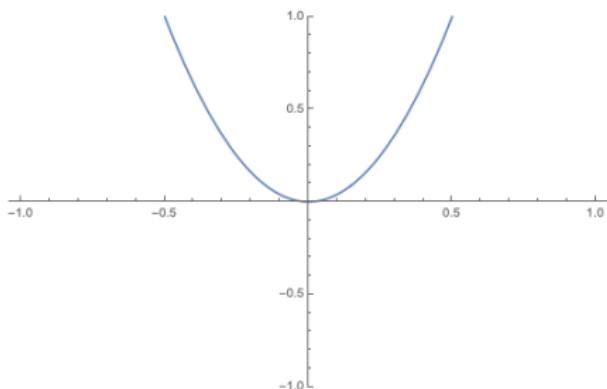
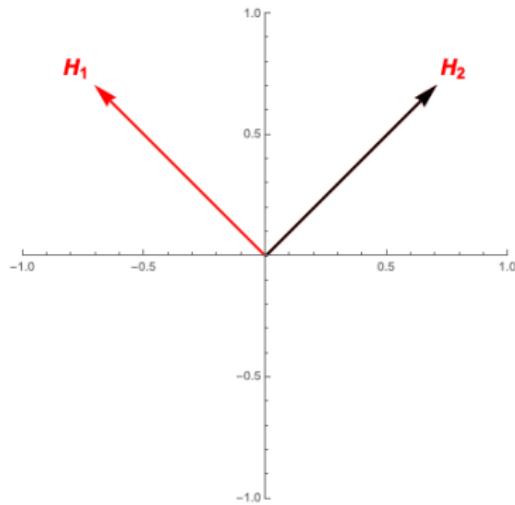
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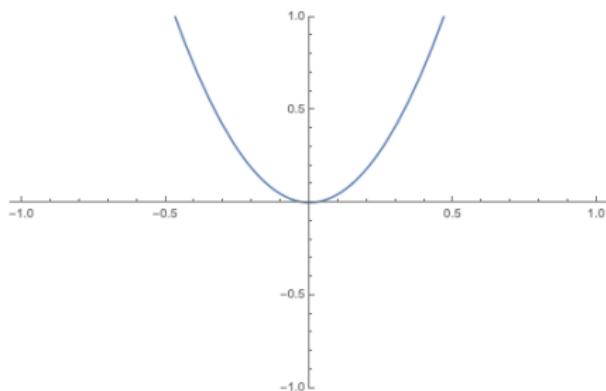
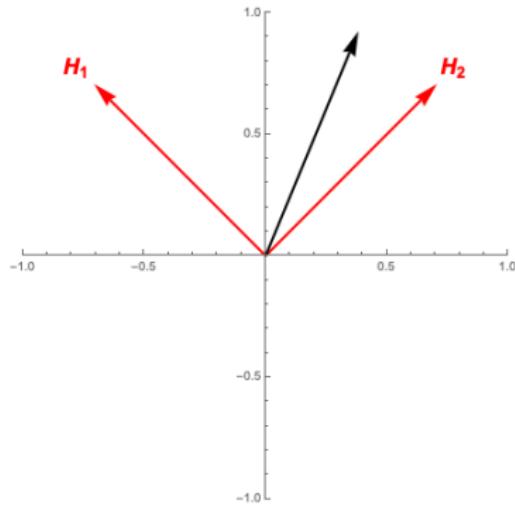
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- $d^T Q d > 0 \forall d$, steepness change with d
- least steep along H_2 ($\lambda_2 = 4$)

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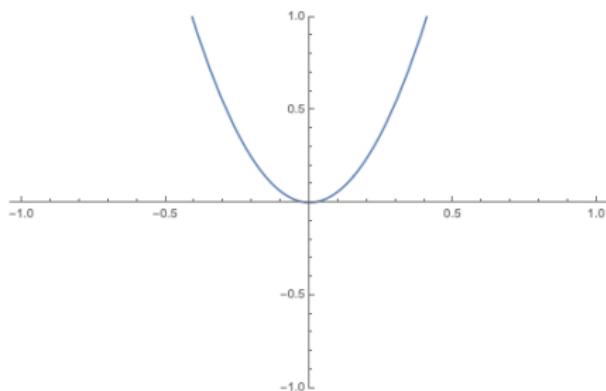
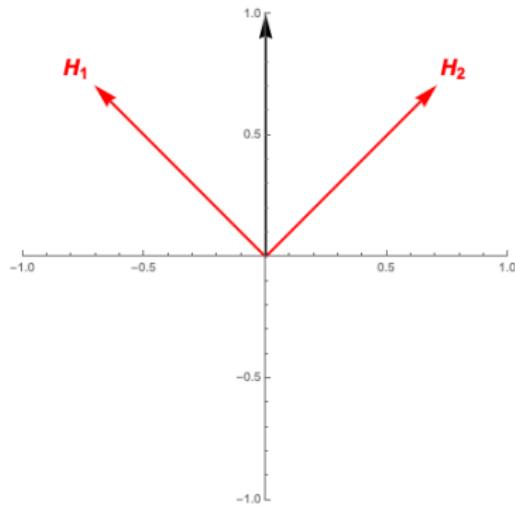


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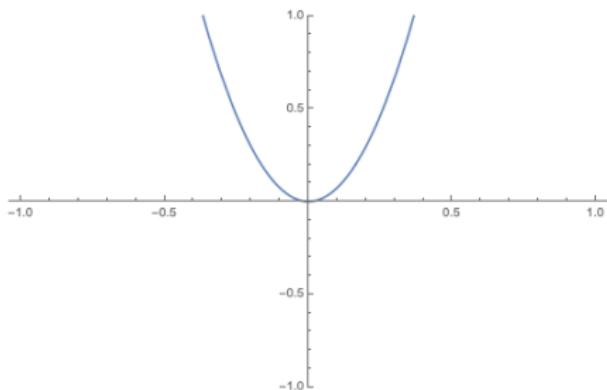
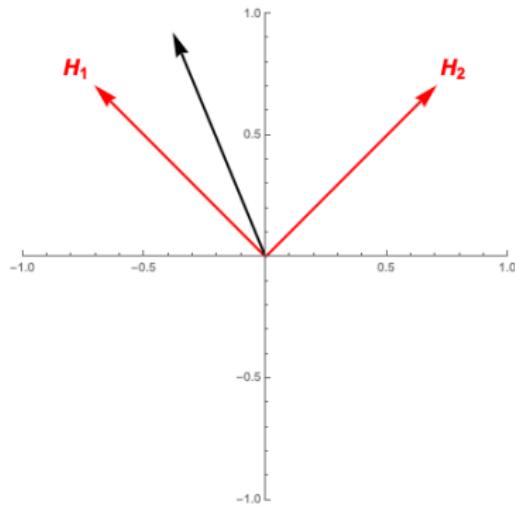


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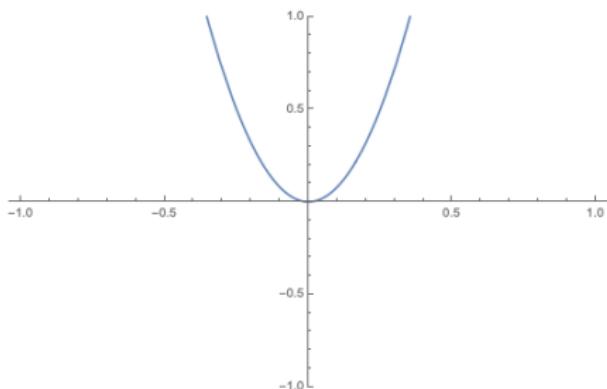
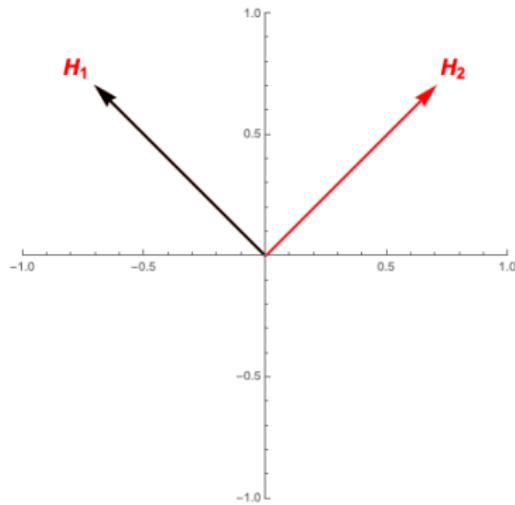


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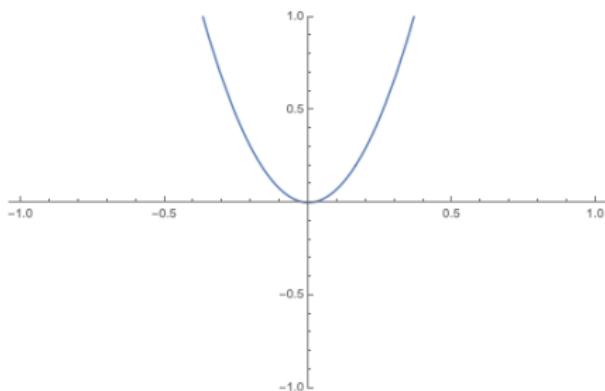
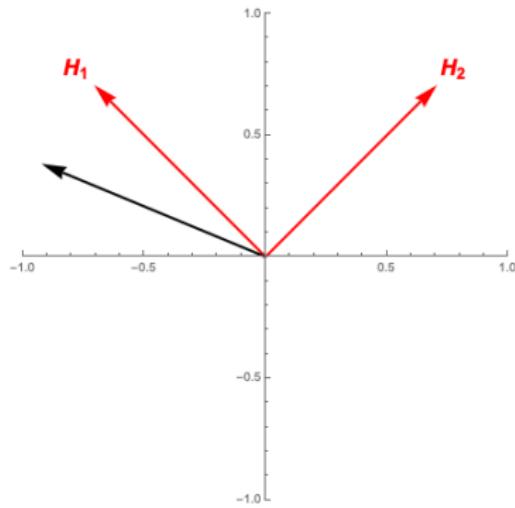
- $Q = \begin{bmatrix} 6 & -2 \\ -2 & 6 \end{bmatrix} \succ 0 \quad H = \frac{\sqrt{2}}{2} \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} \quad \lambda = \begin{bmatrix} 8 \\ 4 \end{bmatrix}$



- $d^T Q d > 0 \forall d$, steepness change with d
- steepest along H_1 ($\lambda_1 = 8$)

- Fundamental relation: $\varphi_{H_i}(\alpha) = \alpha^2 \lambda_i$ (check)

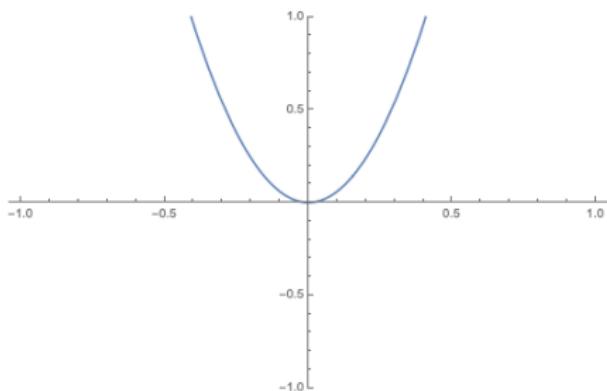
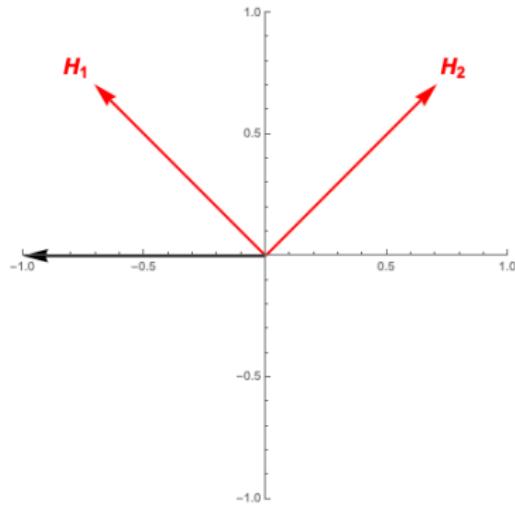
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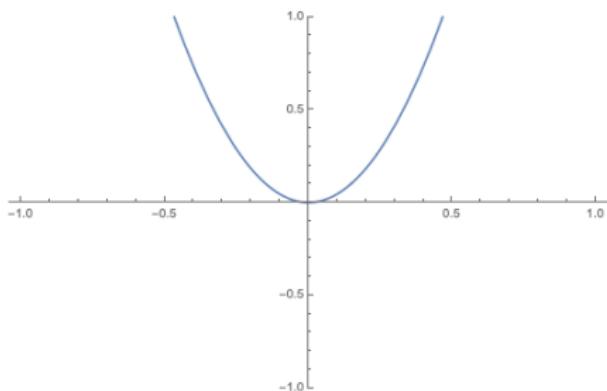
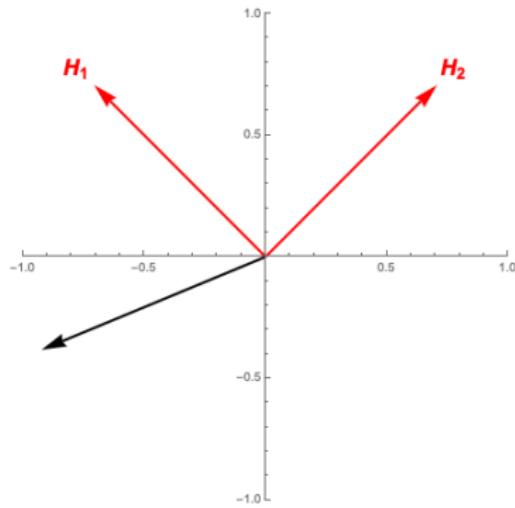
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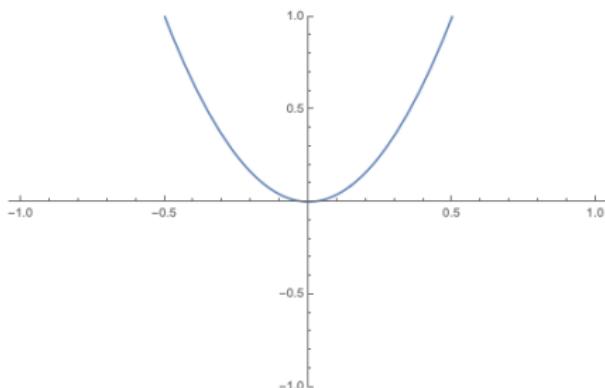
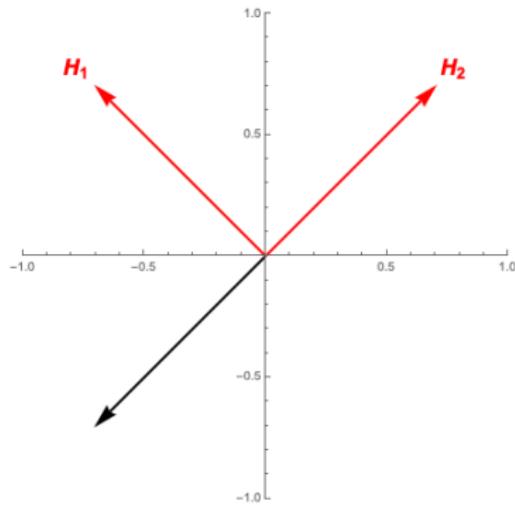
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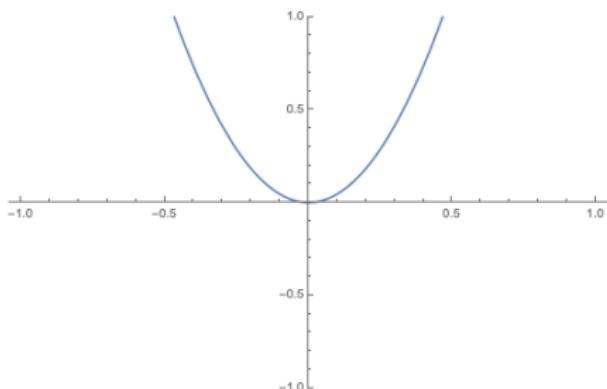
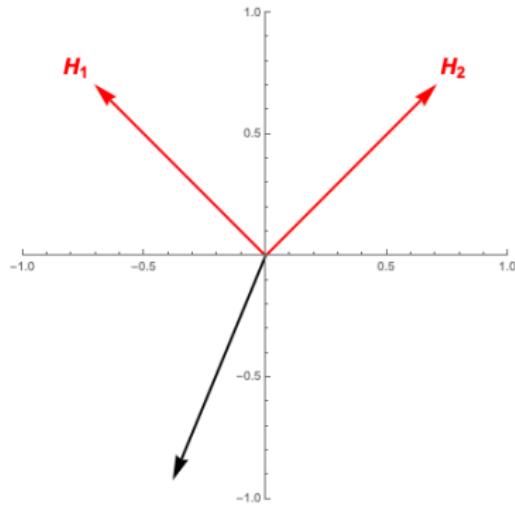
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- $d^T Q d > 0 \forall d$, steepness change with d
- least steep along $-H_2$ ($\lambda_2 = 4$)

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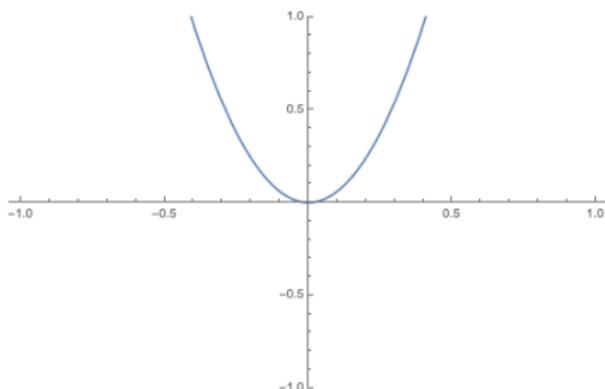
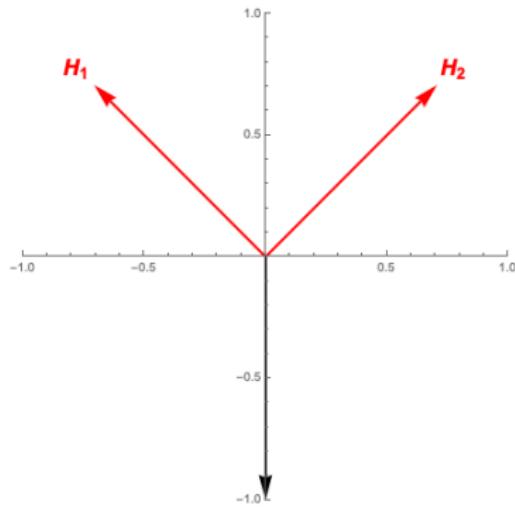
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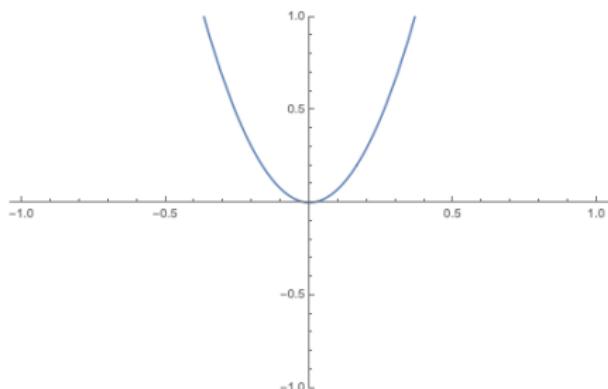
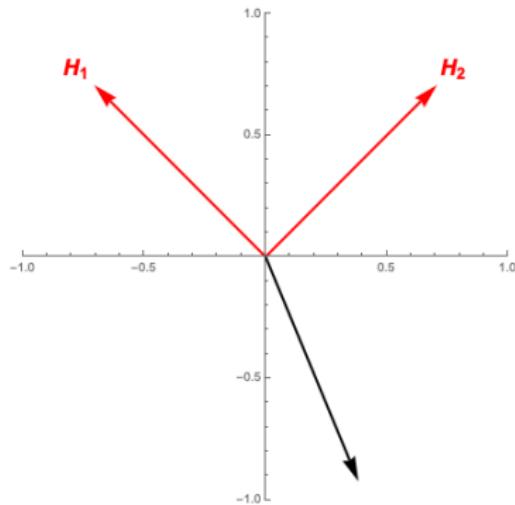
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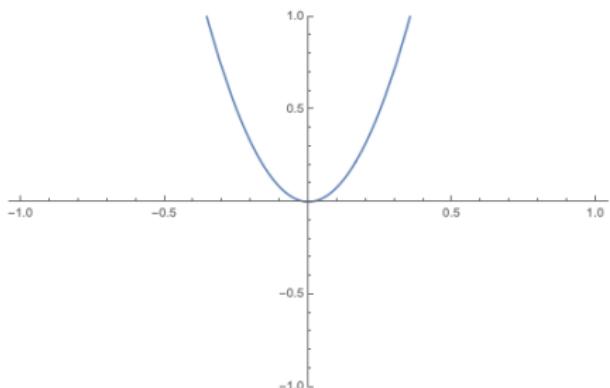
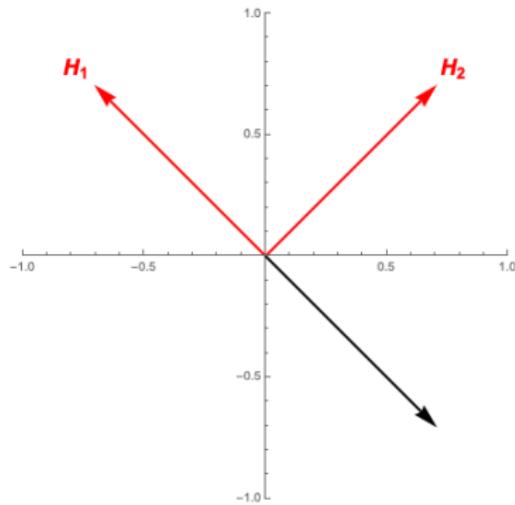
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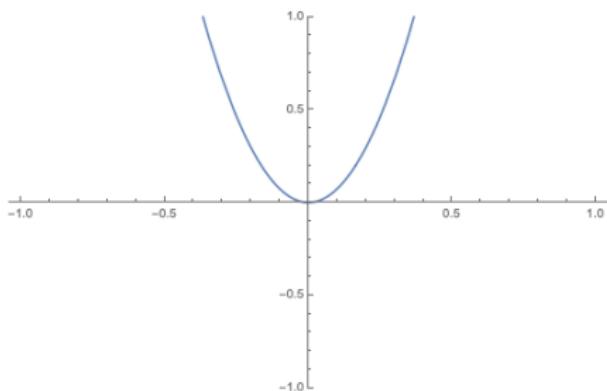
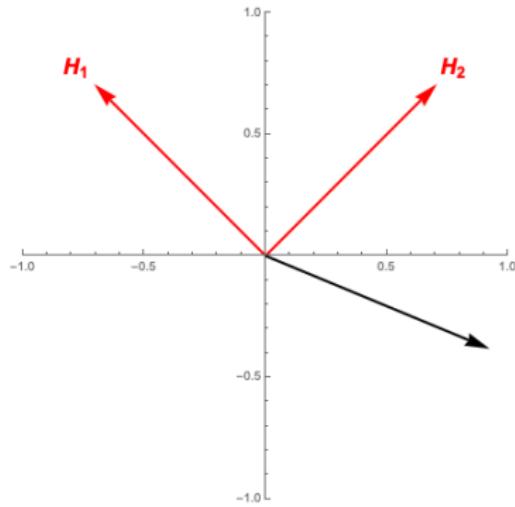
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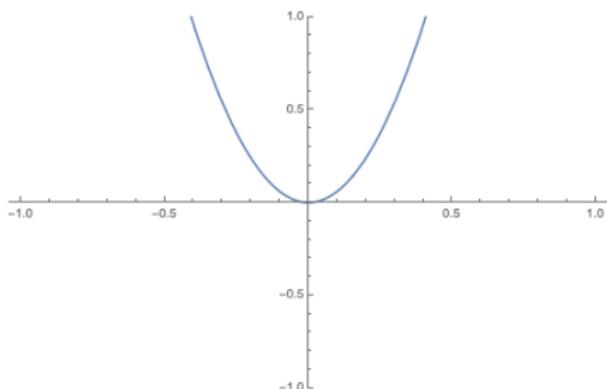
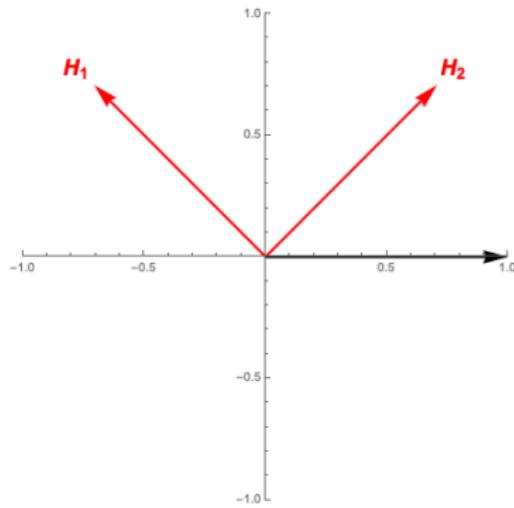
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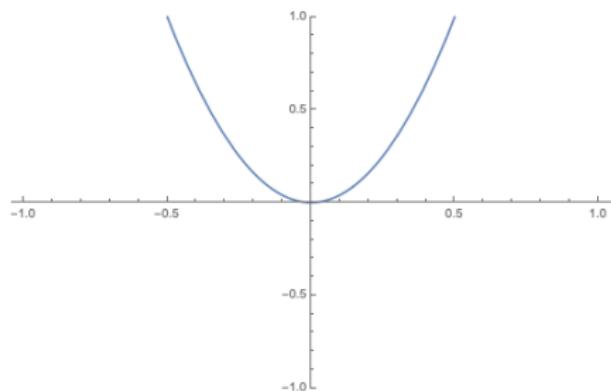
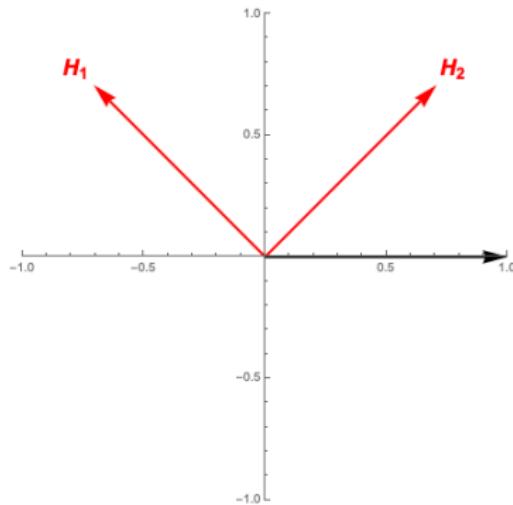
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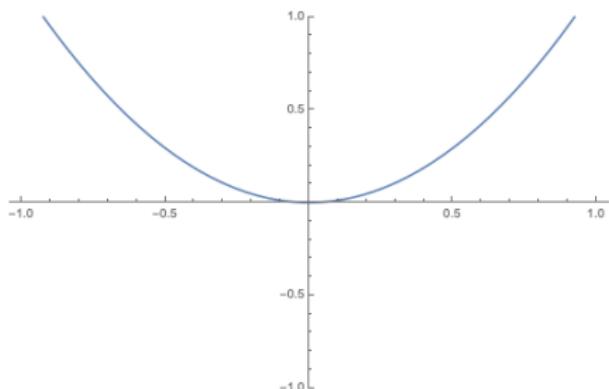
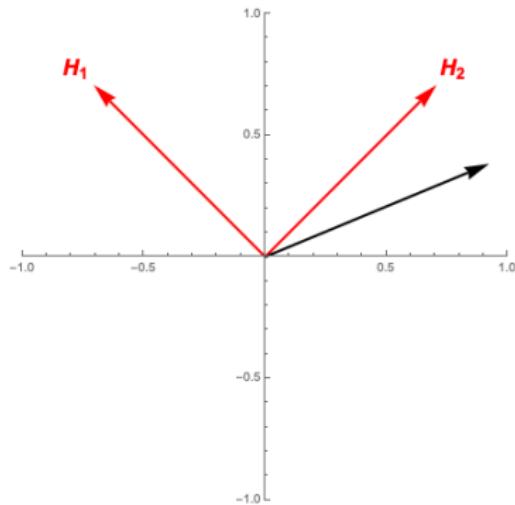
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- ▶

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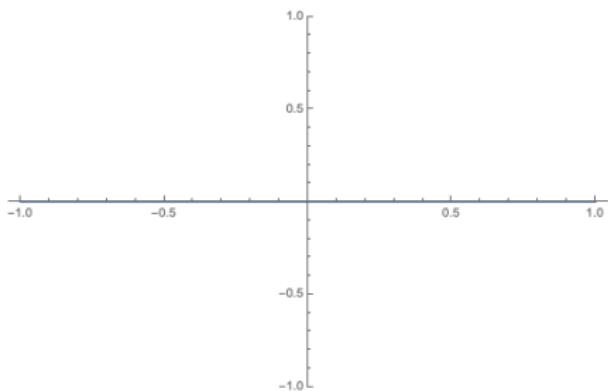
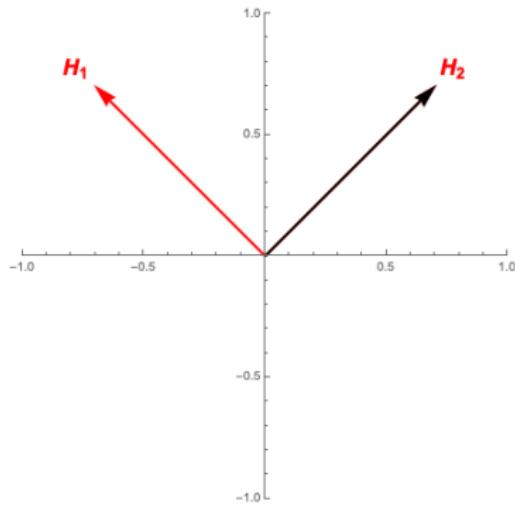
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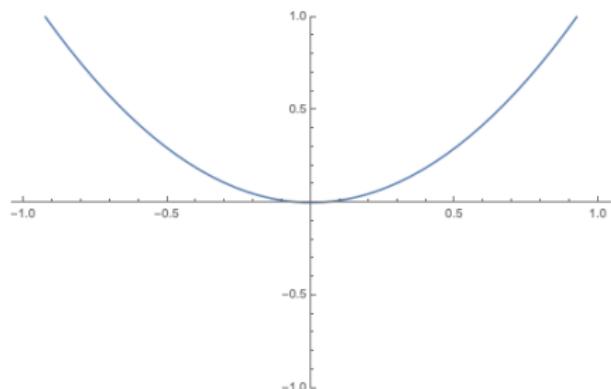
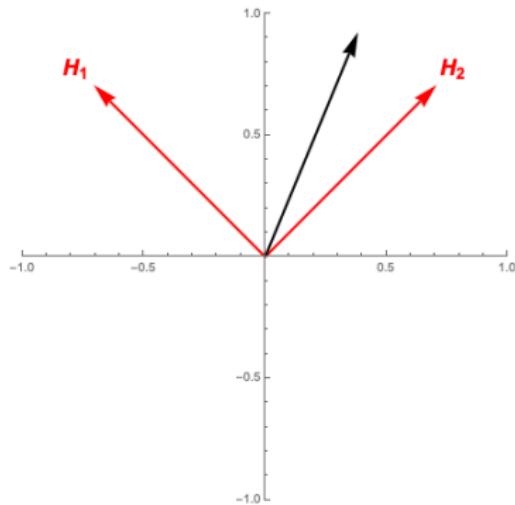
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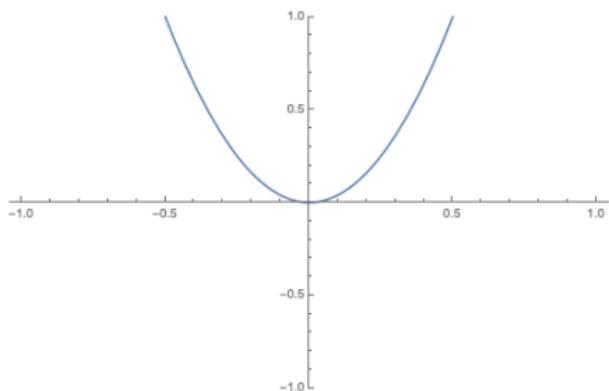
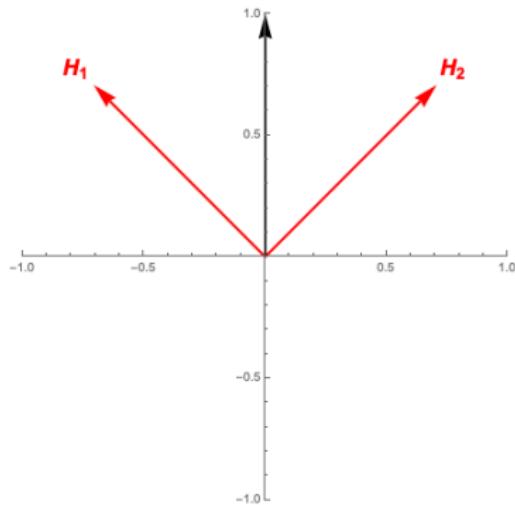


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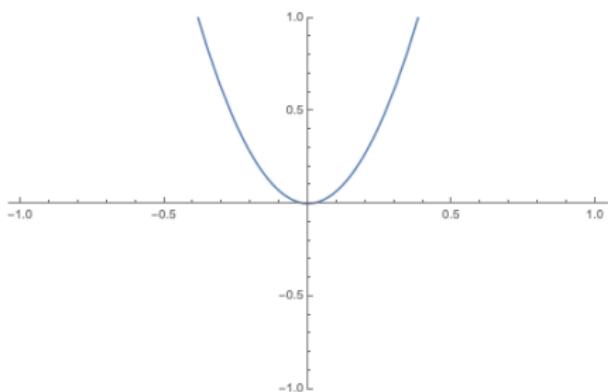
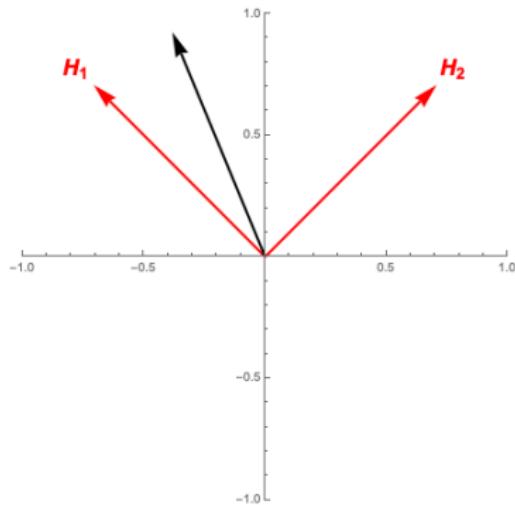


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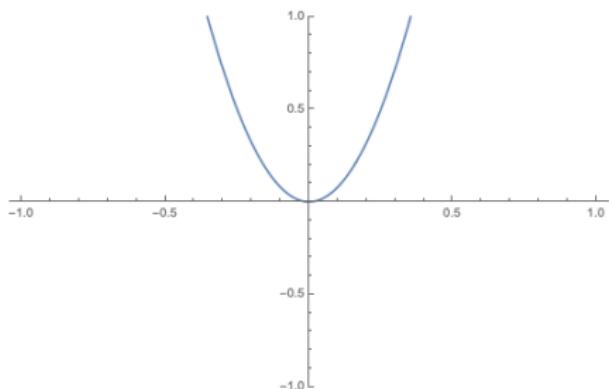
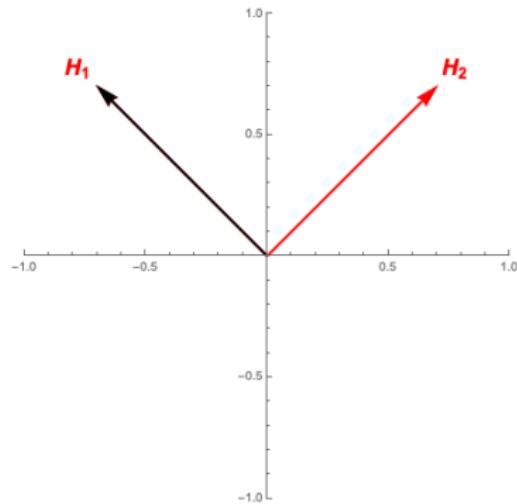
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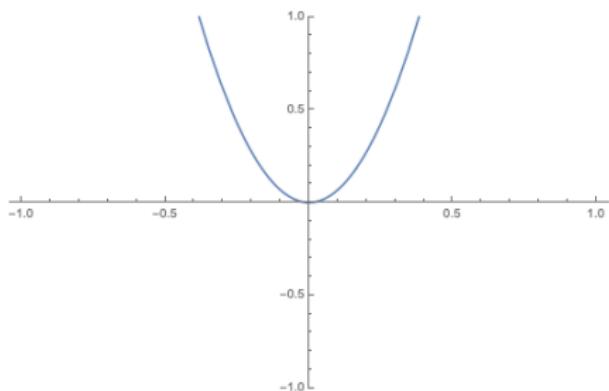
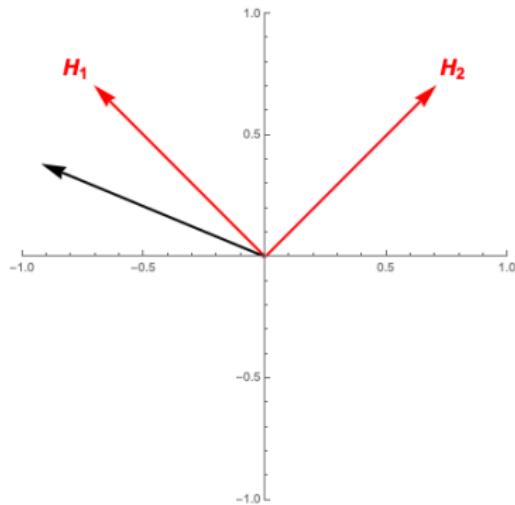
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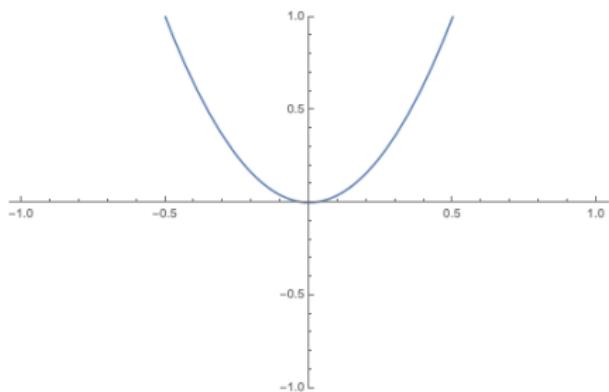
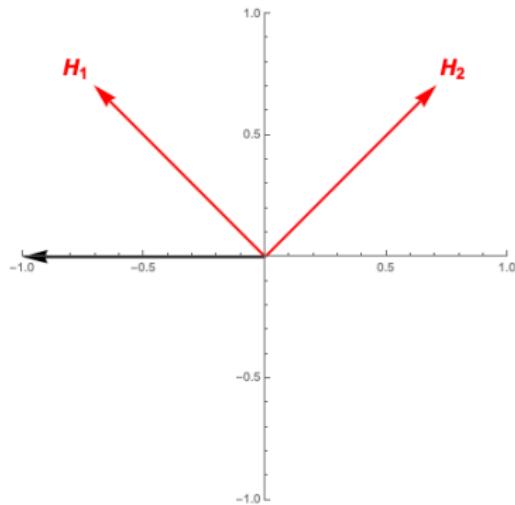
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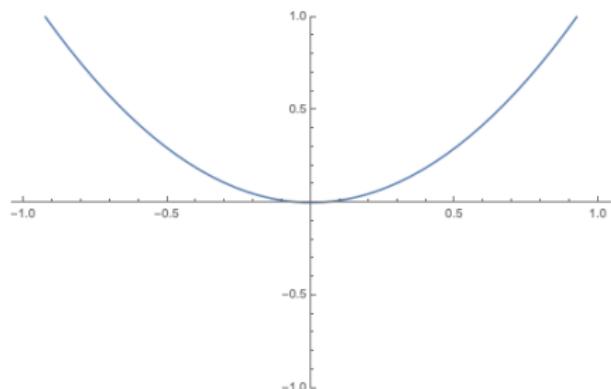
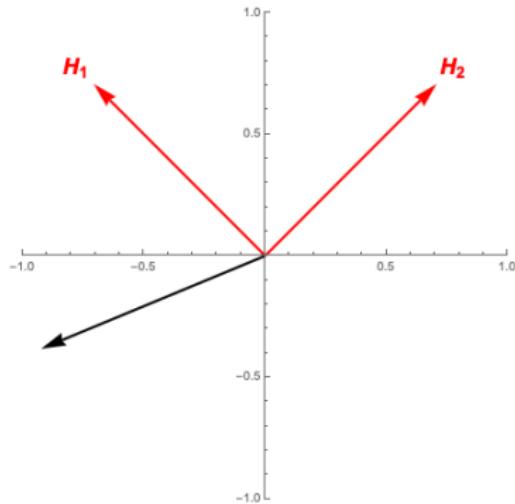
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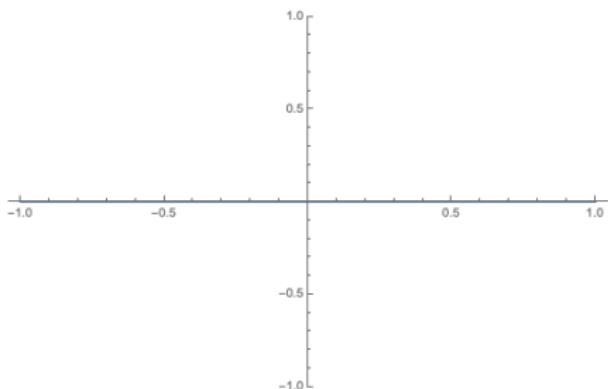
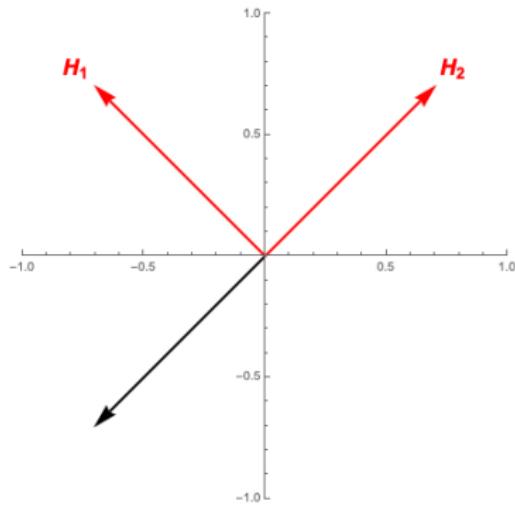
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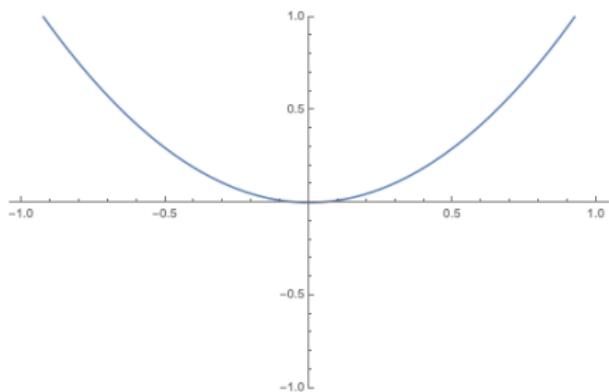
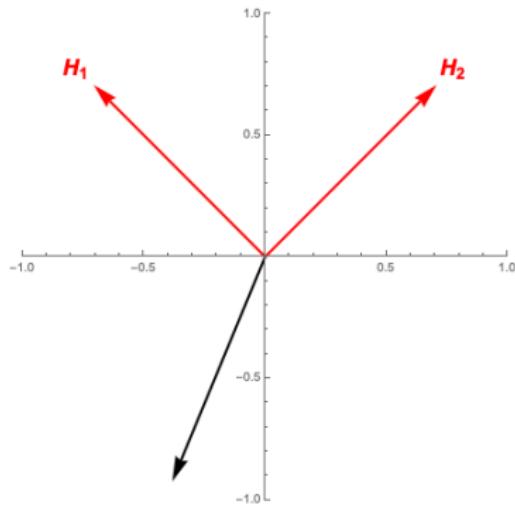
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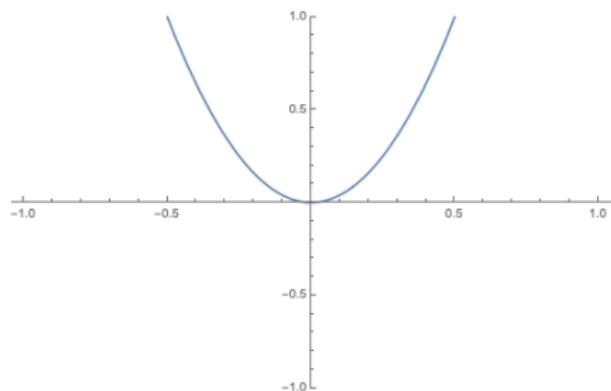
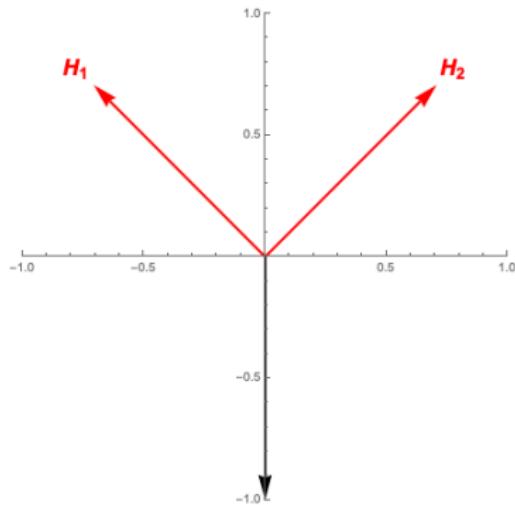
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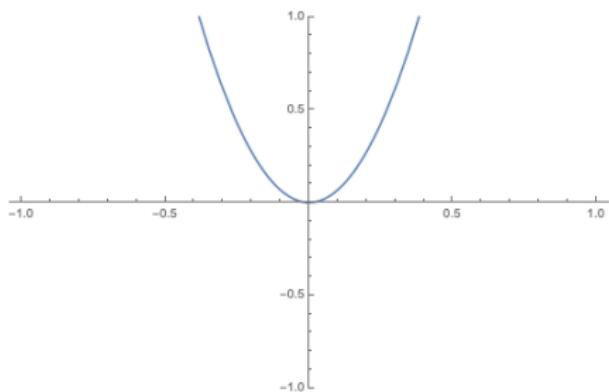
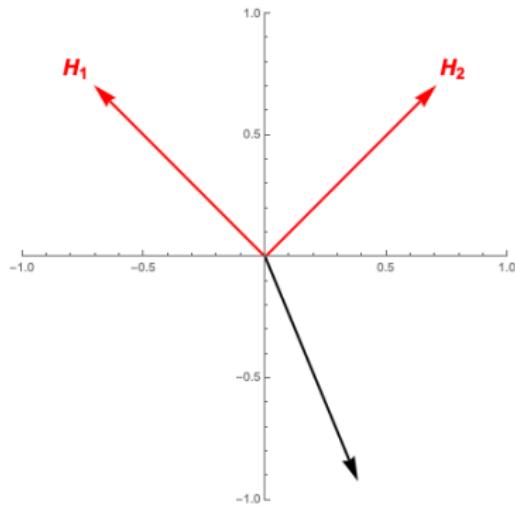
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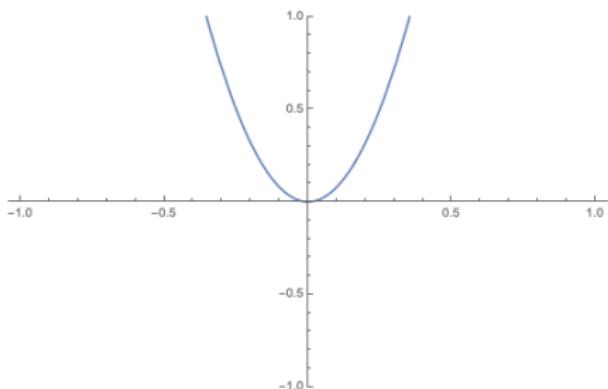
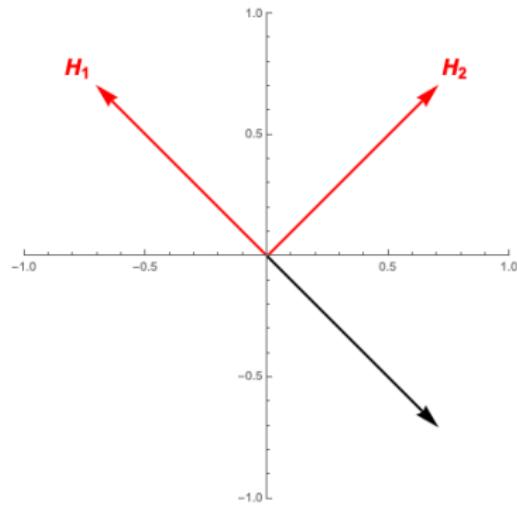
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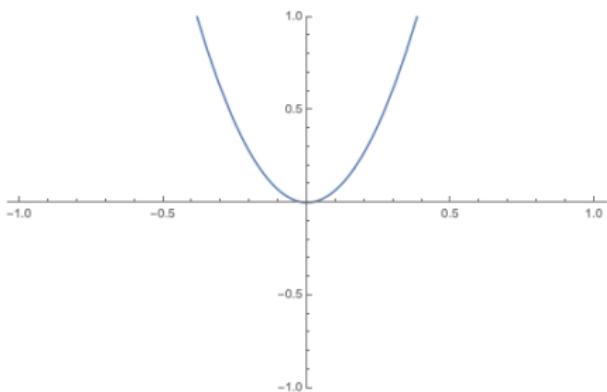
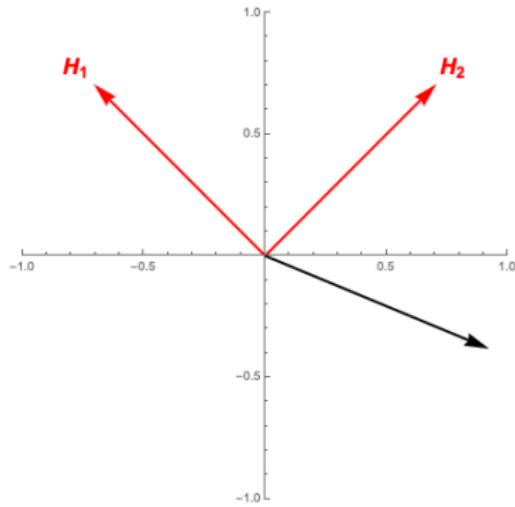
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- ▶ Recall $\varphi_{H_i}(\alpha) = \alpha^2 \lambda_i$

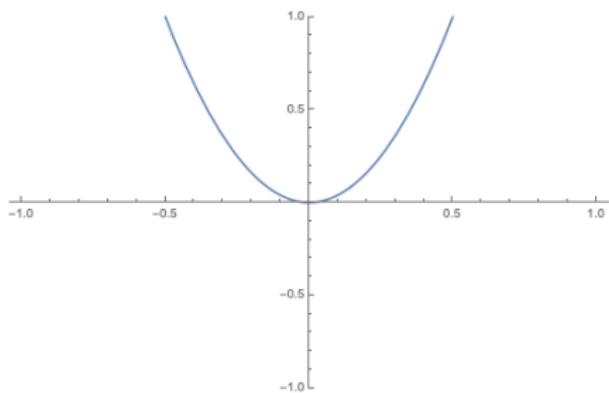
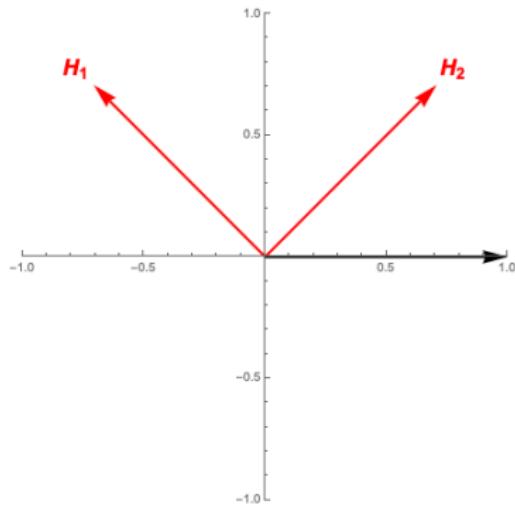
- ▶ $Q = \begin{bmatrix} 4 & -4 \\ -4 & 4 \end{bmatrix} \succeq 0 \quad H = \frac{\sqrt{2}}{2} \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} \quad \lambda = \begin{bmatrix} 8 \\ 0 \end{bmatrix}$



- ▶ $d^T Q d \geq 0 \forall d$, but $\exists d$ s.t. $d^T Q d = 0$
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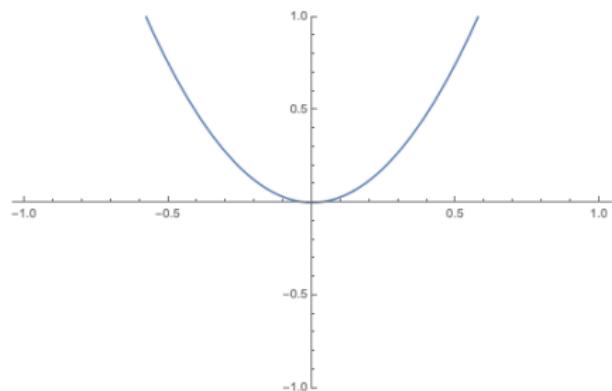
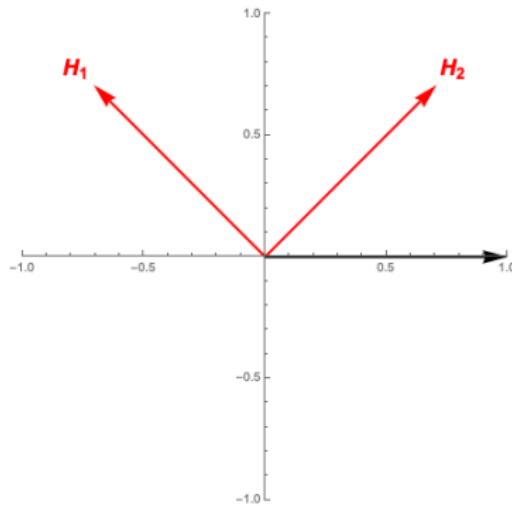
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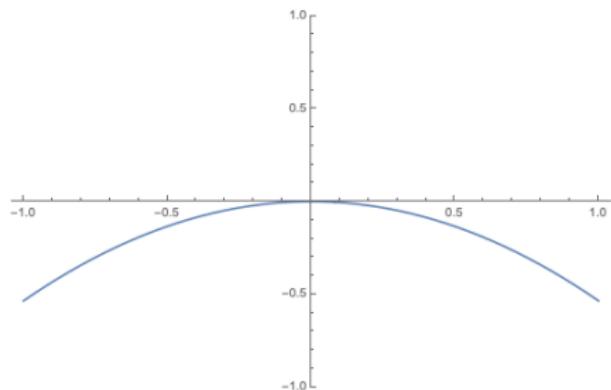
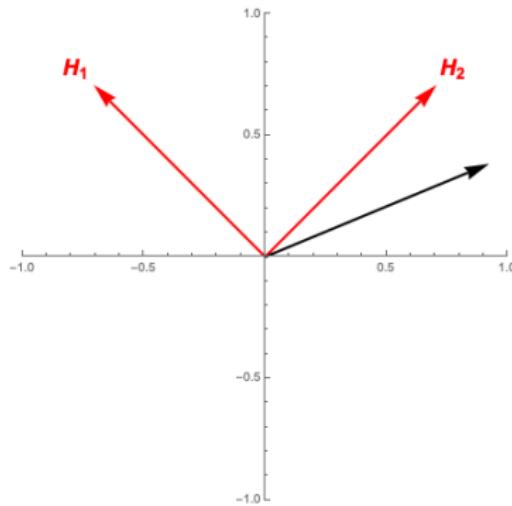
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- ▶ $d^T Q d$ can be both > 0 and < 0
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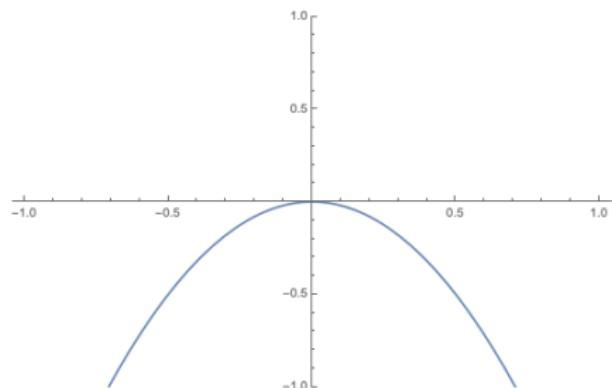
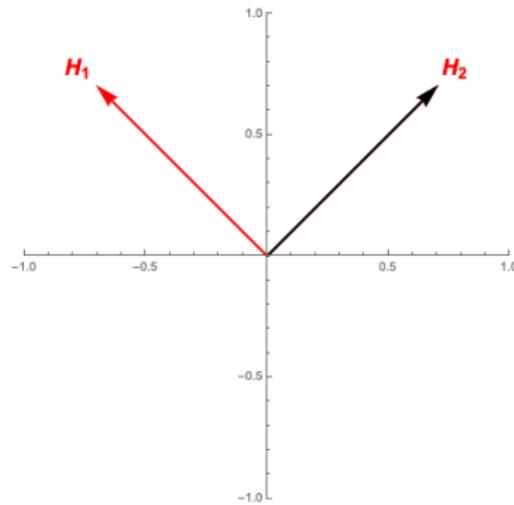


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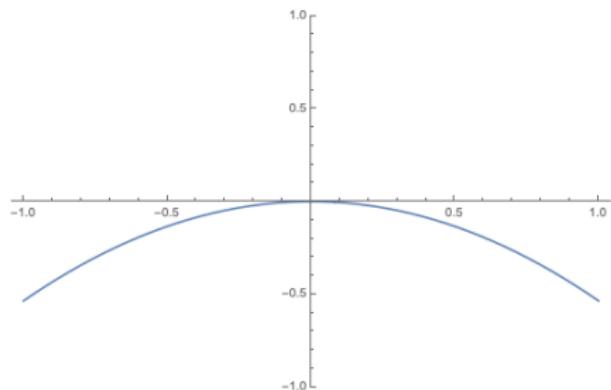
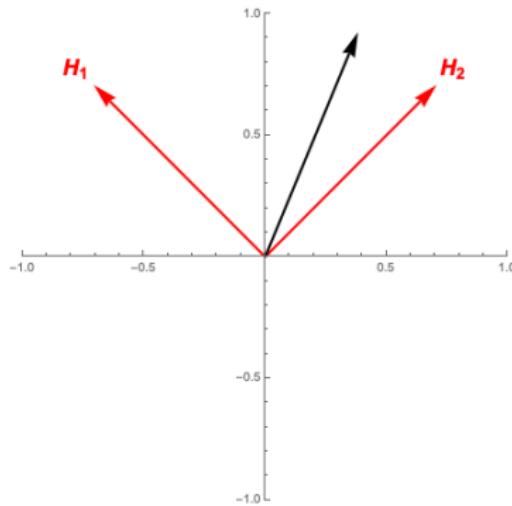
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- ▶ $d^T Q d$ can be both > 0 and < 0
- ▶ steepest negative along H_2 ($\lambda_2 = -2$)

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- ▶ $Q = \begin{bmatrix} 3 & -5 \\ -5 & 3 \end{bmatrix} \asymp 0 \quad H = \frac{\sqrt{2}}{2} \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} \quad \lambda = \begin{bmatrix} 8 \\ -2 \end{bmatrix}$

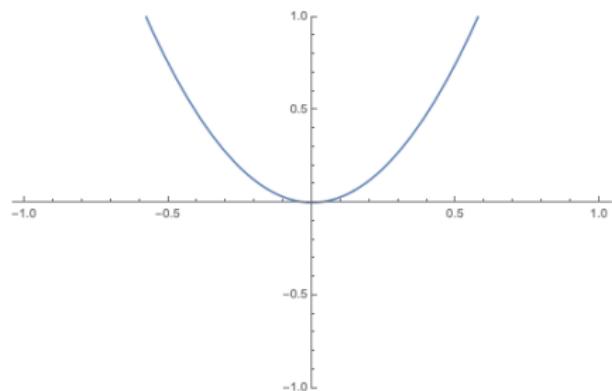
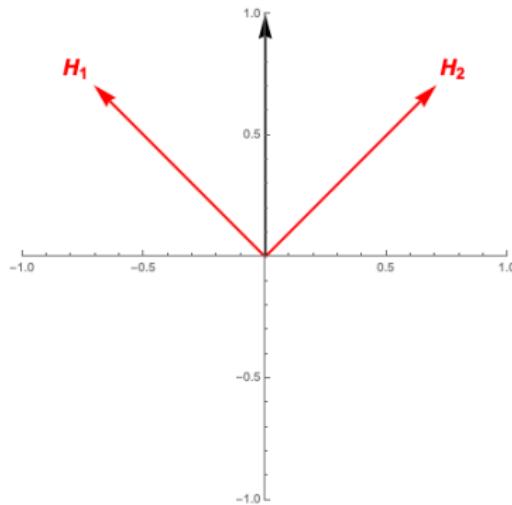


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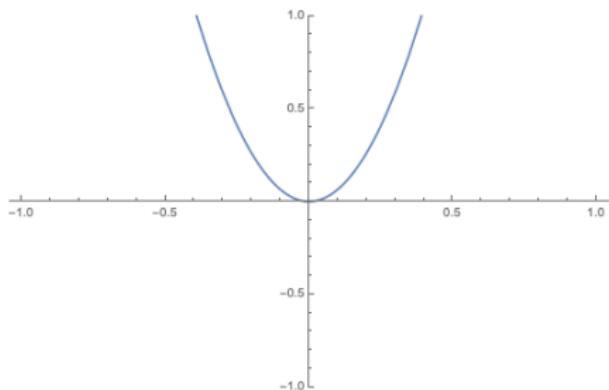
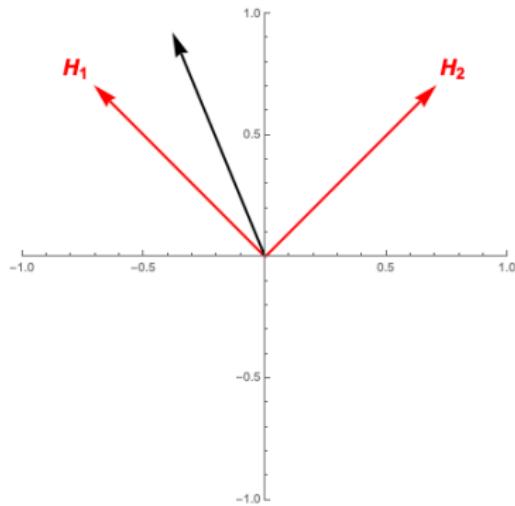


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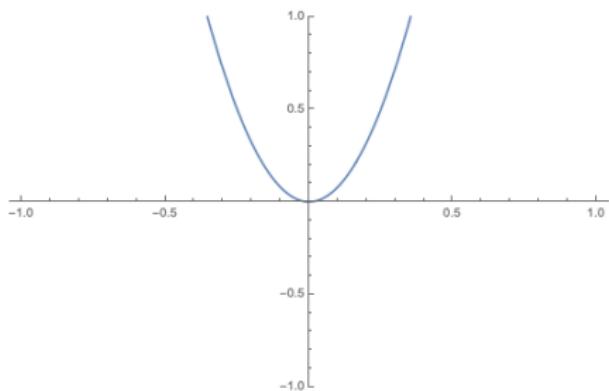
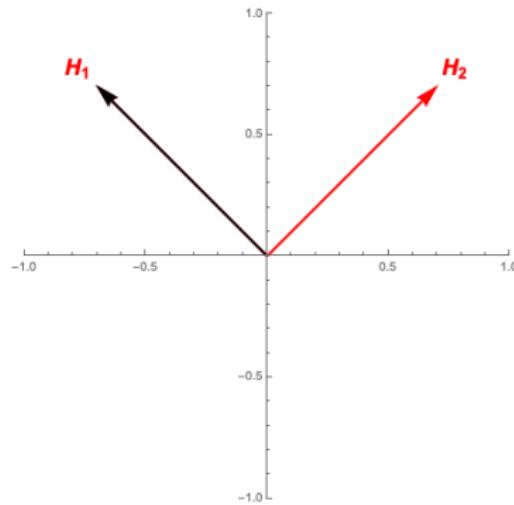
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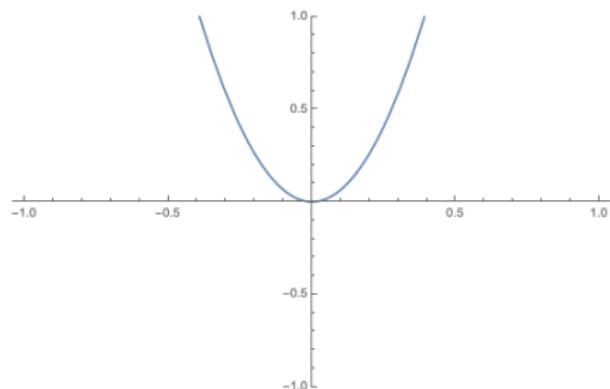
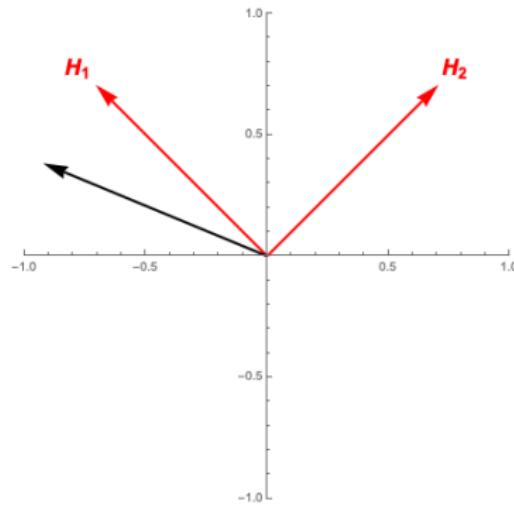
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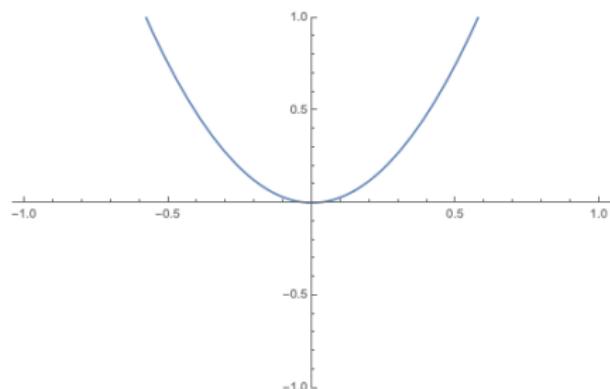
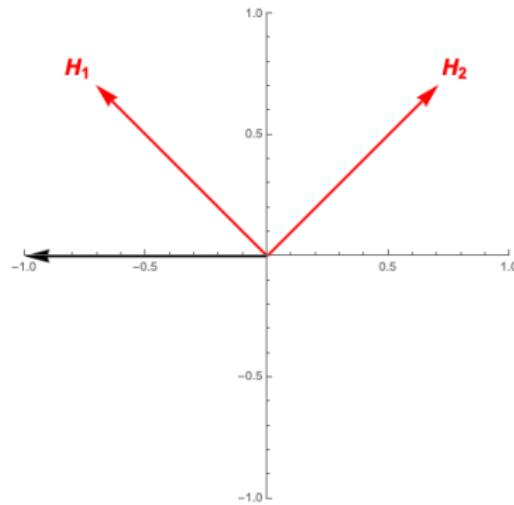
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- ▶ $d^T Q d$ can be both > 0 and < 0
- ▶ intermediate steepness (positive or negative) “in between”

- ▶ Recall $\varphi_{H_i}(\alpha) = \alpha^2 \lambda_i$

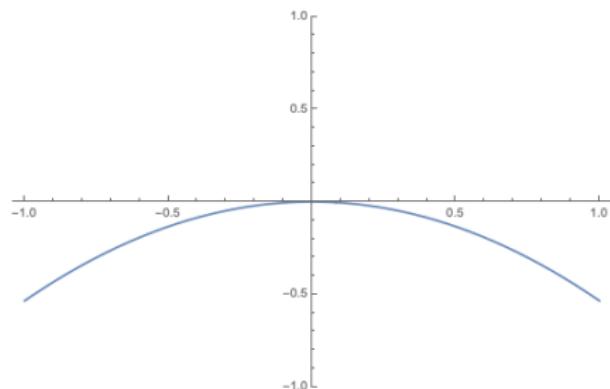
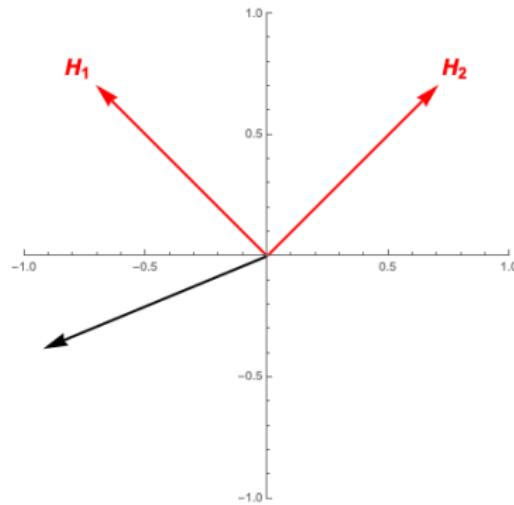
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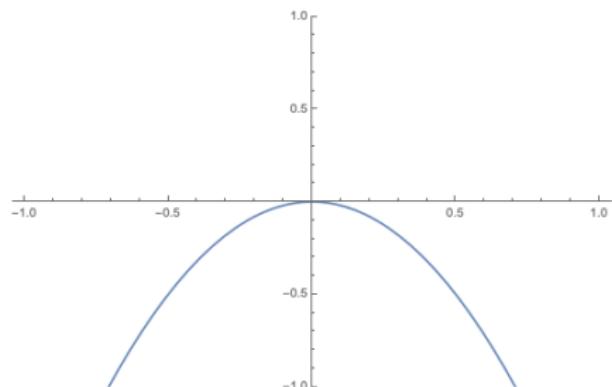
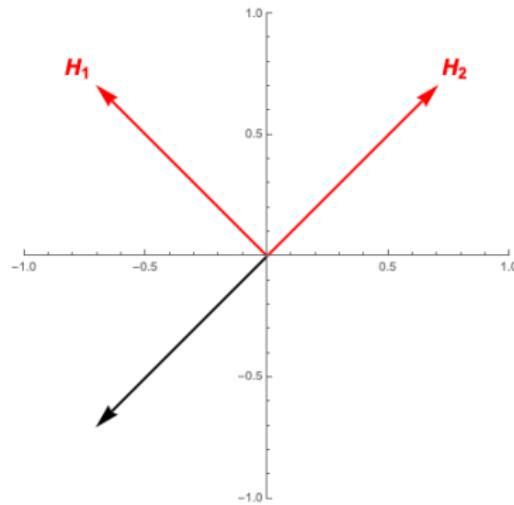
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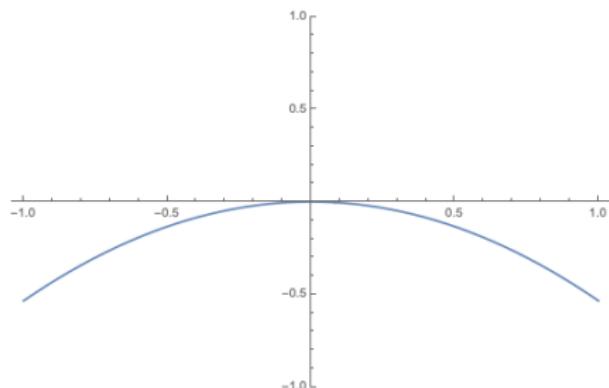
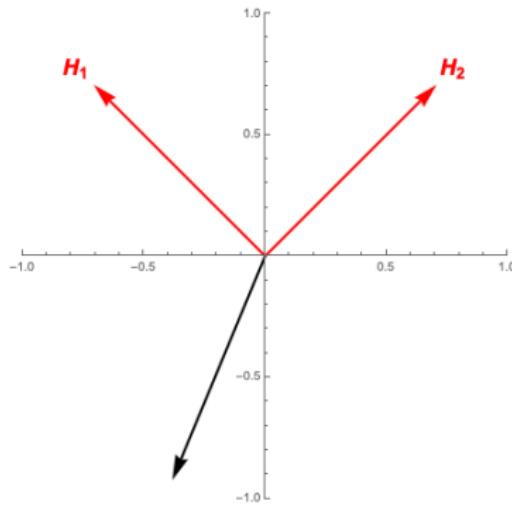
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- ▶ $d^T Q d$ can be both > 0 and < 0
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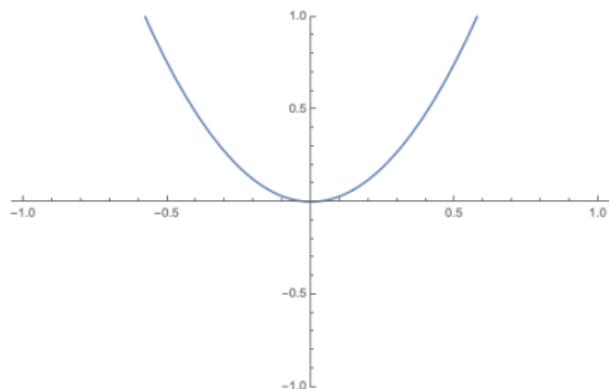
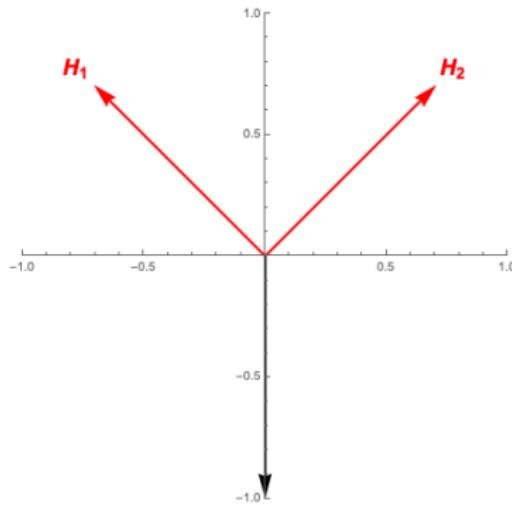
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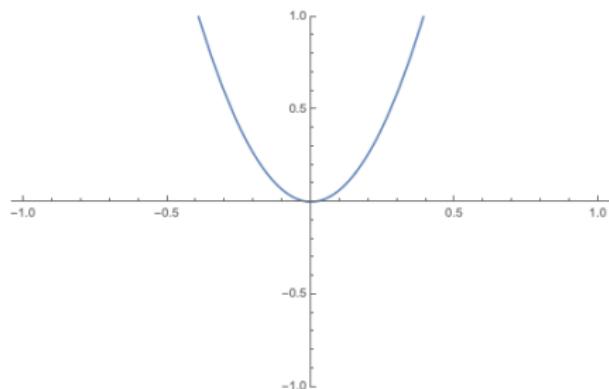
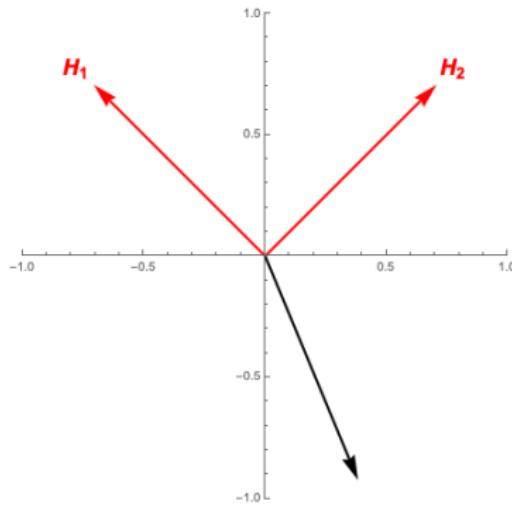
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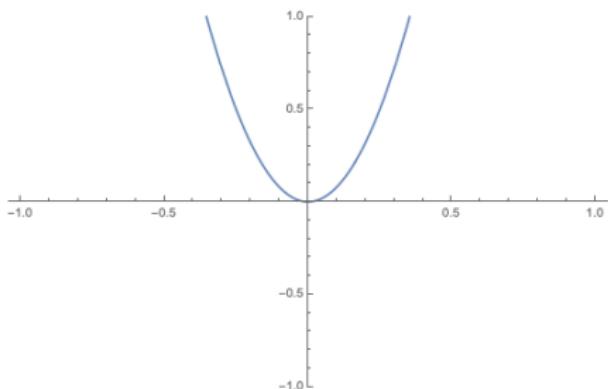
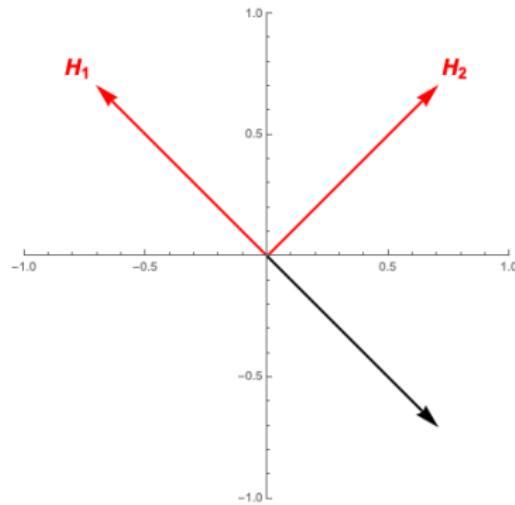
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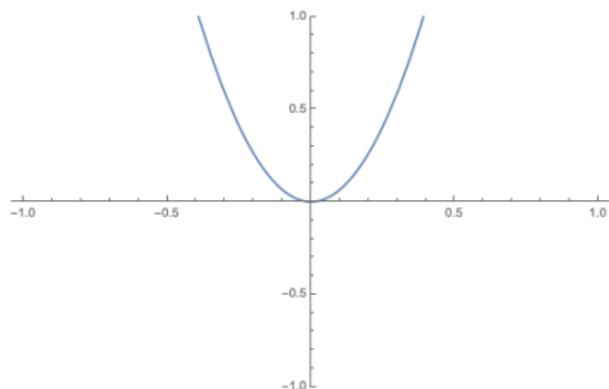
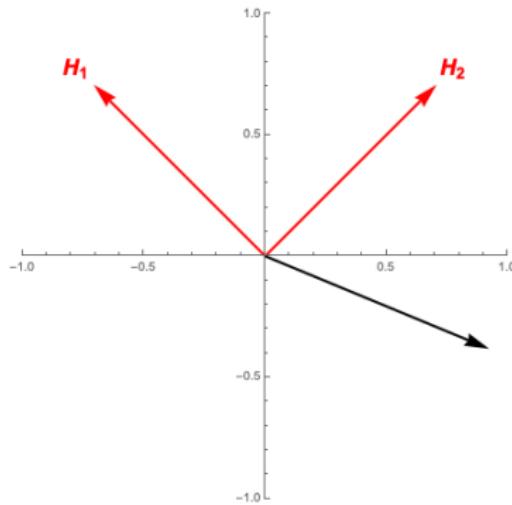
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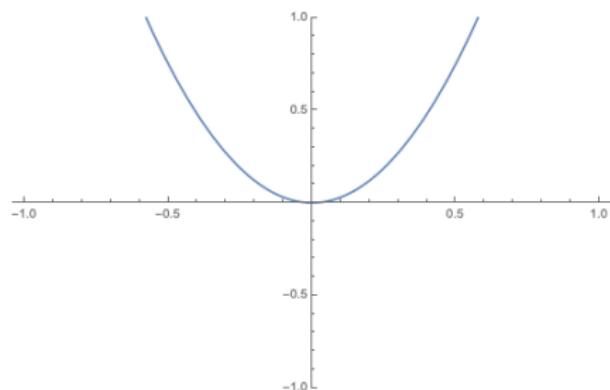
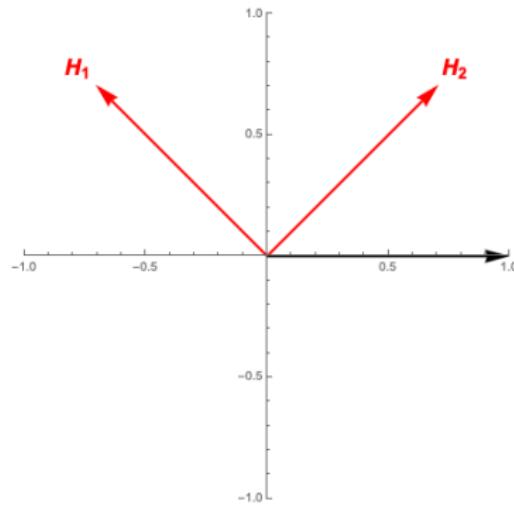
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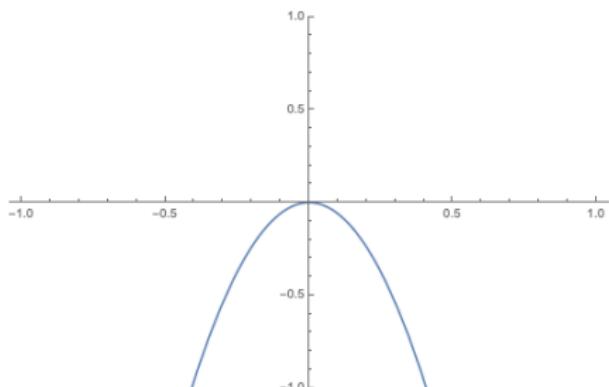
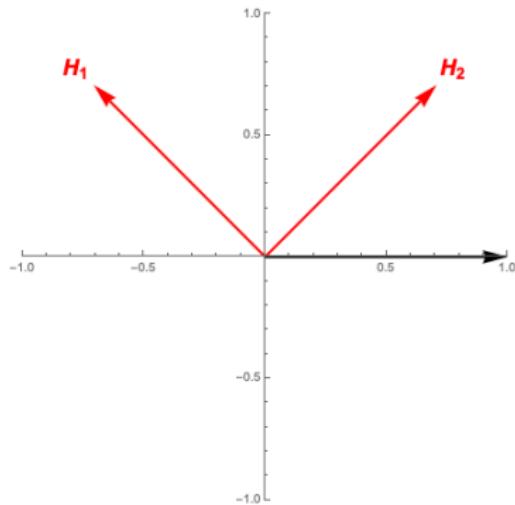
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- ▶ $Q = \begin{bmatrix} -6 & -2 \\ -2 & -6 \end{bmatrix} \prec 0 \quad H = \frac{\sqrt{2}}{2} \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} \quad \lambda = \begin{bmatrix} -4 \\ -8 \end{bmatrix}$

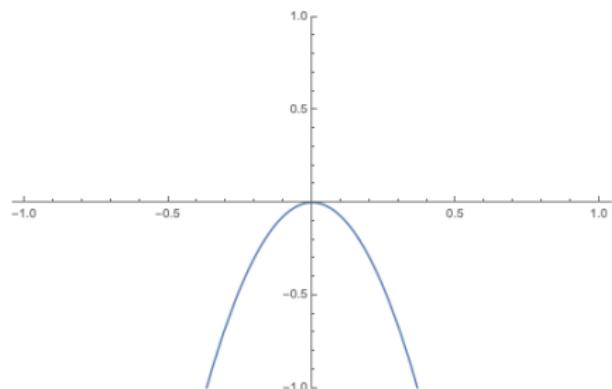
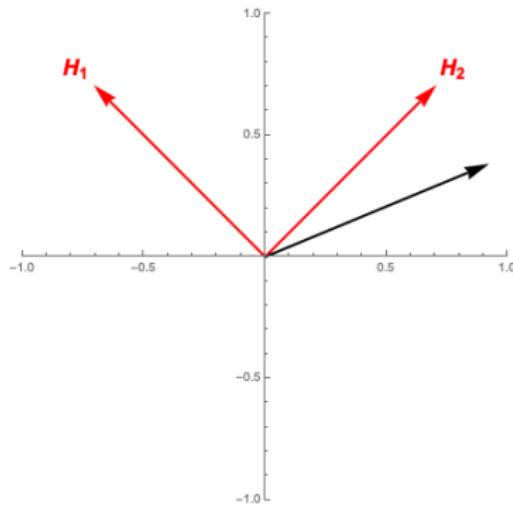


- ▶ $d^T Q d < 0 \forall d$, steepness change with d



- ▶ Recall $\varphi_{H_i}(\alpha) = \alpha^2 \lambda_i$

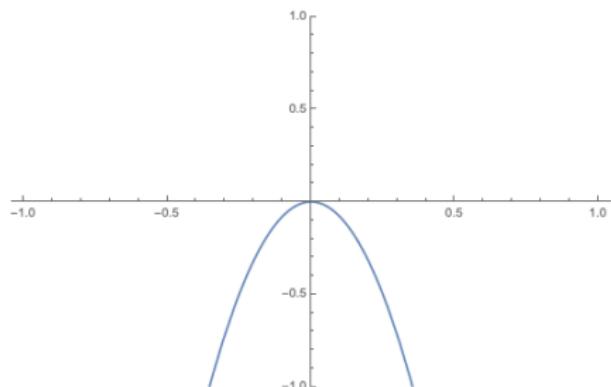
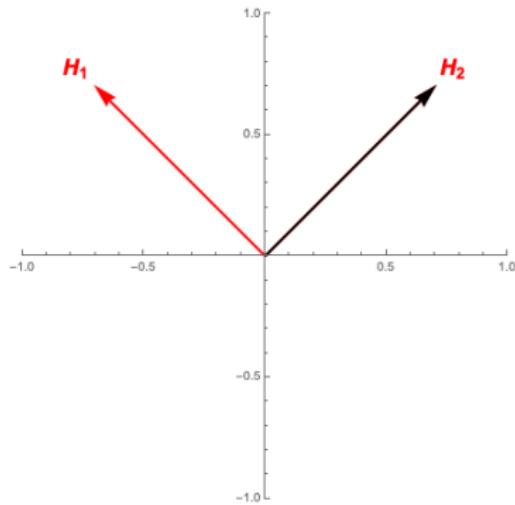
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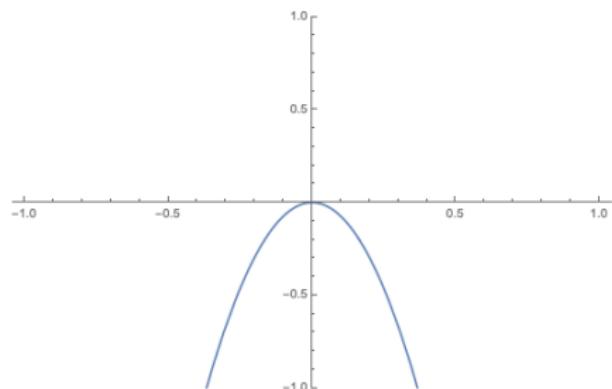
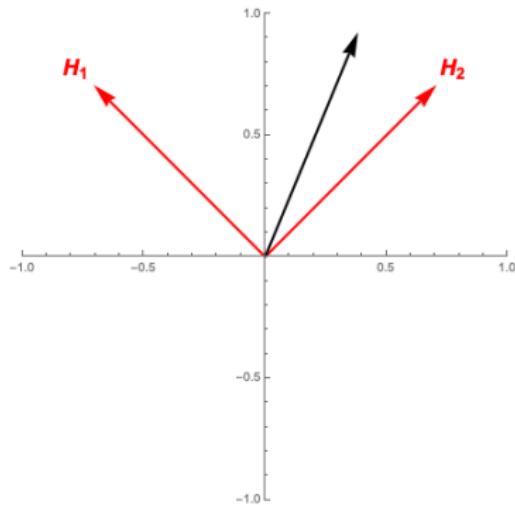
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- ▶ $d^T Q d < 0 \forall d$, steepness change with d
- ▶ steepest negative along H_2 ($\lambda_2 = -8$)

- ▶ Recall $\varphi_{H_i}(\alpha) = \alpha^2 \lambda_i$

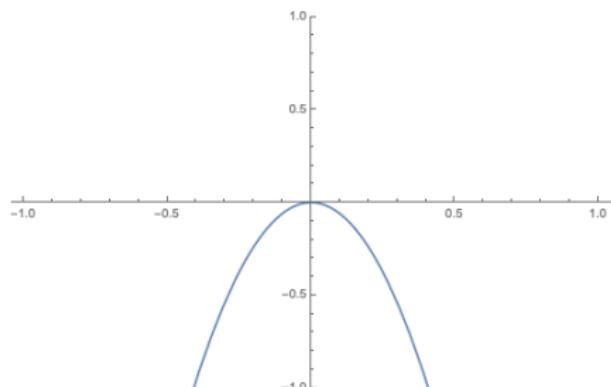
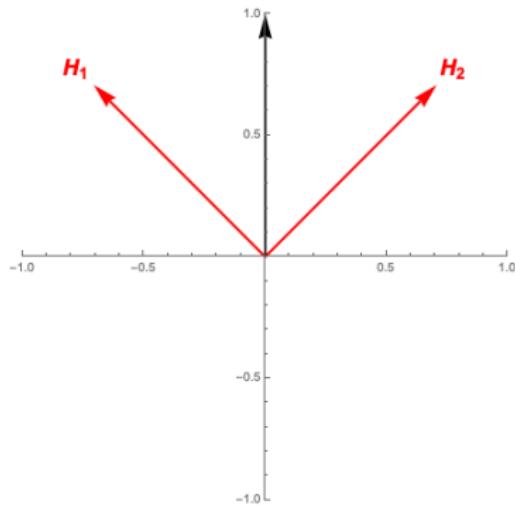
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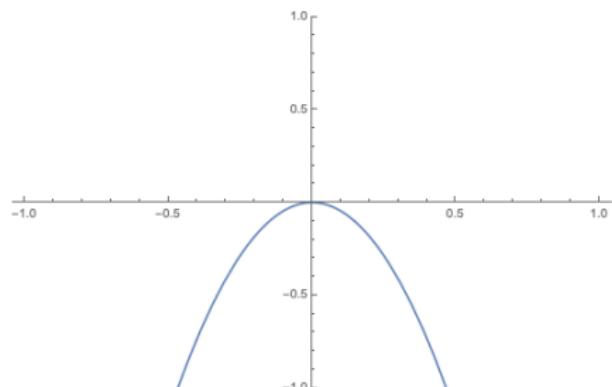
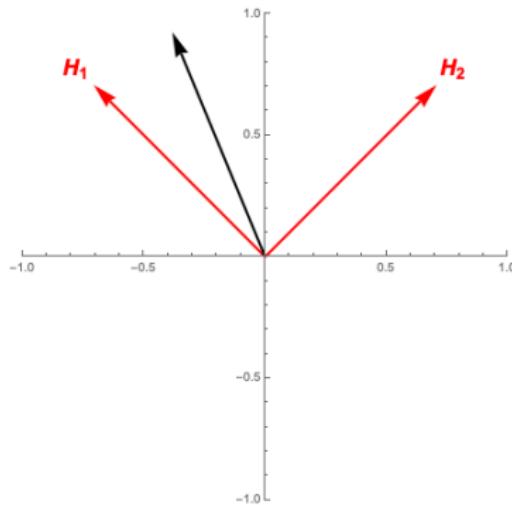


- ▶ $d^T Q d < 0 \forall d$, steepness change with d



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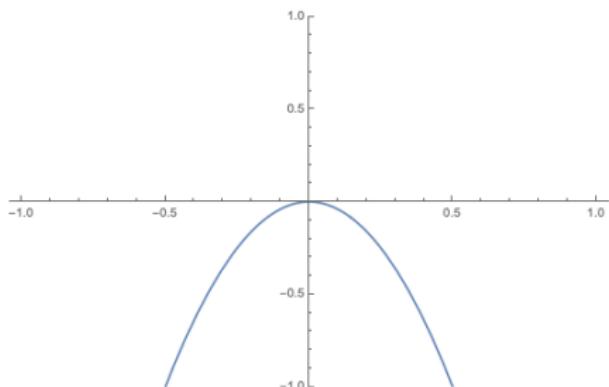
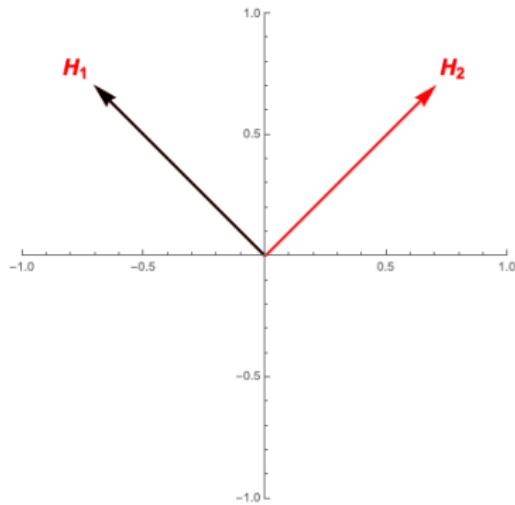


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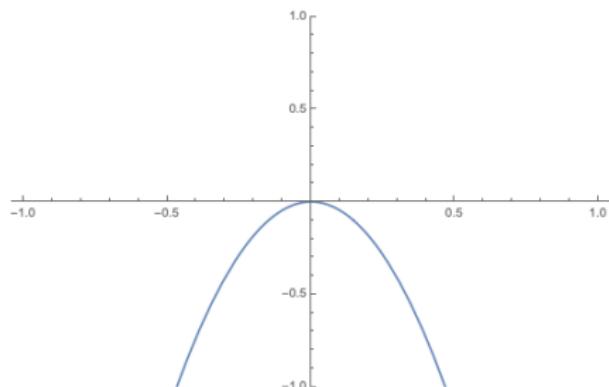
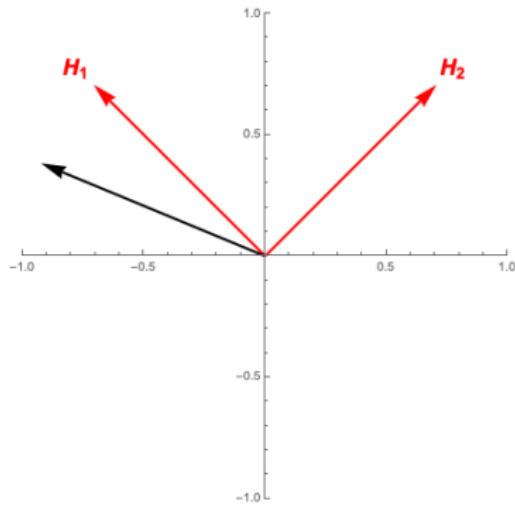
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- ▶ $d^T Q d < 0 \forall d$, steepness change with d
- ▶ least steep negative along H_1 ($\lambda_1 = -4$)

- ▶ Recall $\varphi_{H_i}(\alpha) = \alpha^2 \lambda_i$

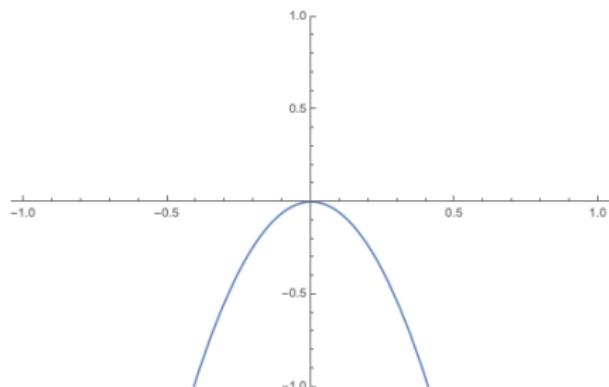
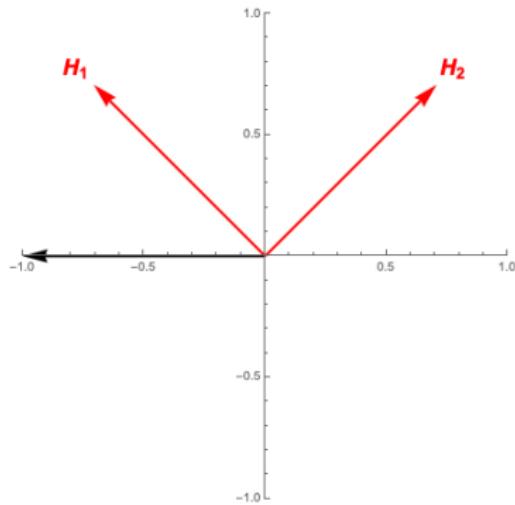
- ▶ $Q = \begin{bmatrix} -6 & -2 \\ -2 & -6 \end{bmatrix} \prec 0 \quad H = \frac{\sqrt{2}}{2} \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} \quad \lambda = \begin{bmatrix} -4 \\ -8 \end{bmatrix}$



- ▶ $d^T Q d < 0 \forall d$, steepness change with d
- ▶ intermediate steepness (negative) “in between”

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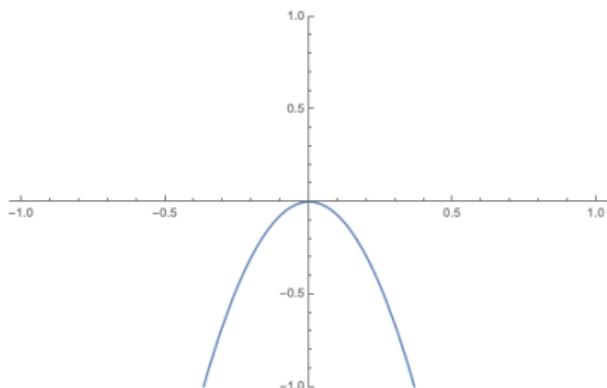
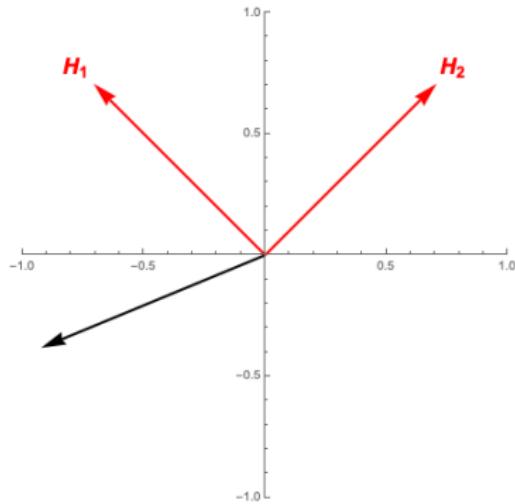
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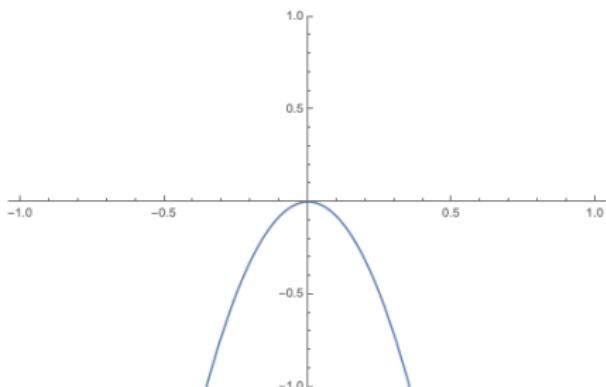
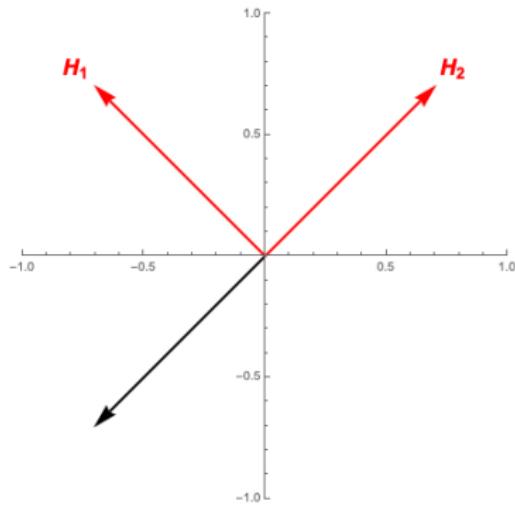
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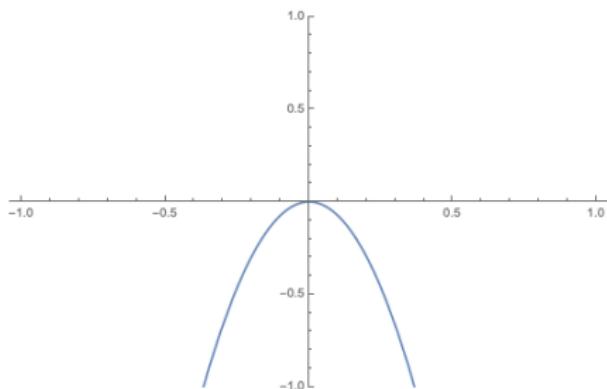
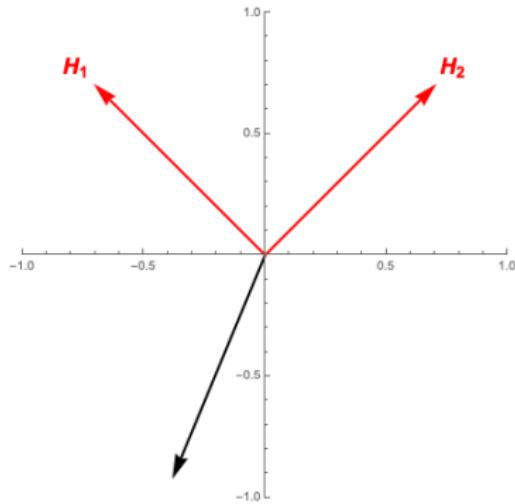
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- ▶ $d^T Q d < 0 \forall d$, steepness change with d
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- ▶ Recall $\varphi_{H_i}(\alpha) = \alpha^2 \lambda_i$

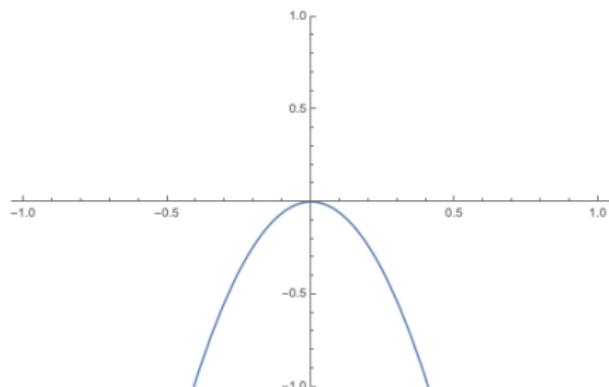
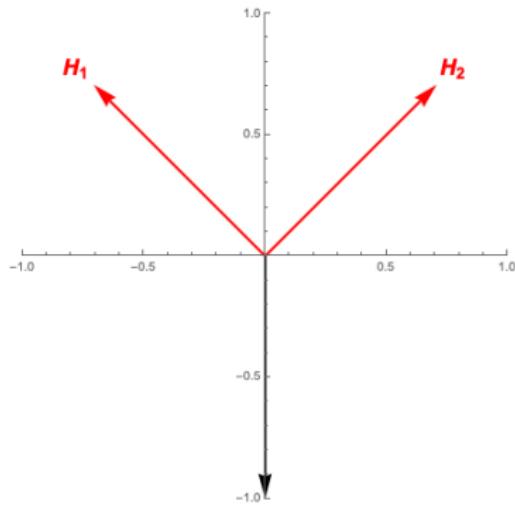
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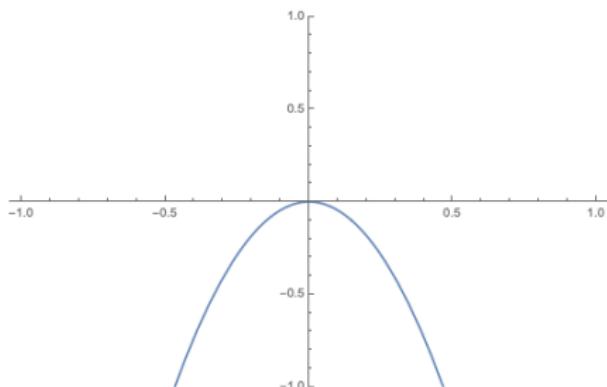
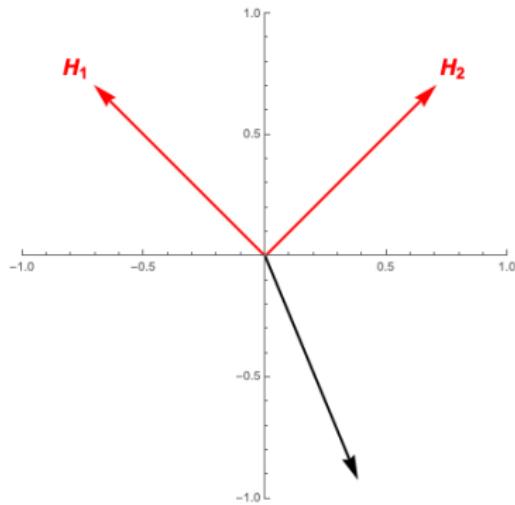
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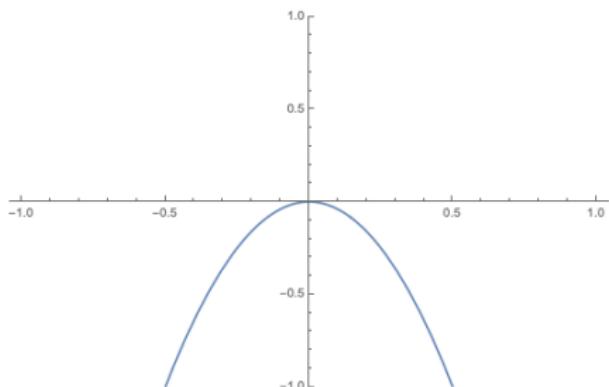
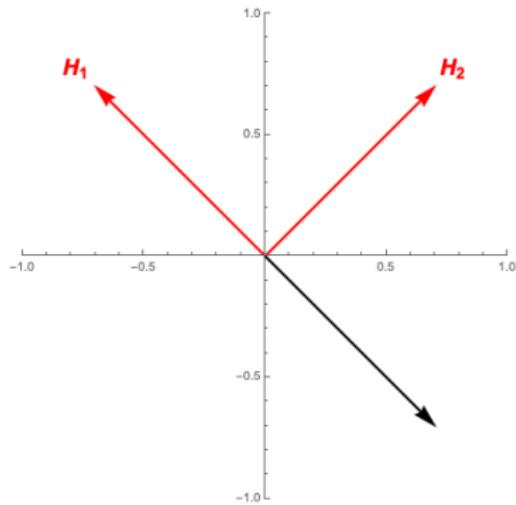
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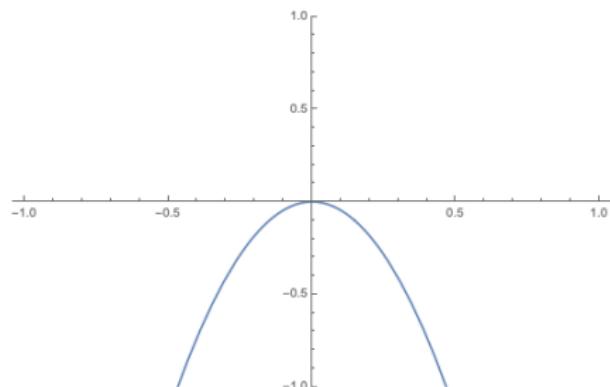
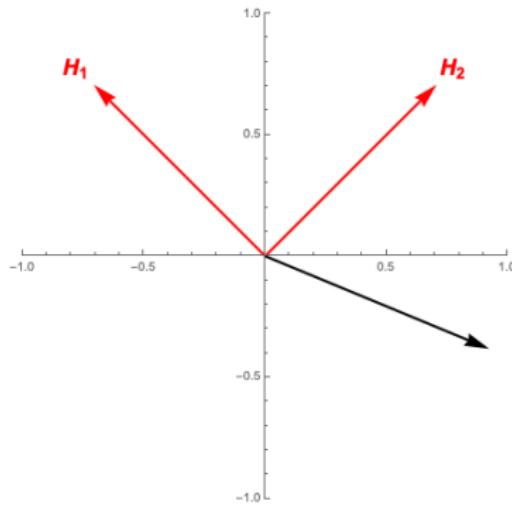
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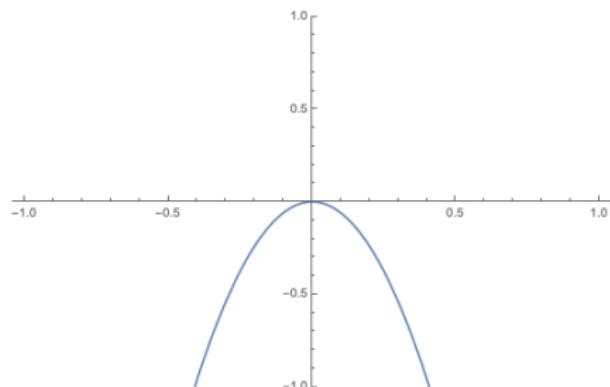
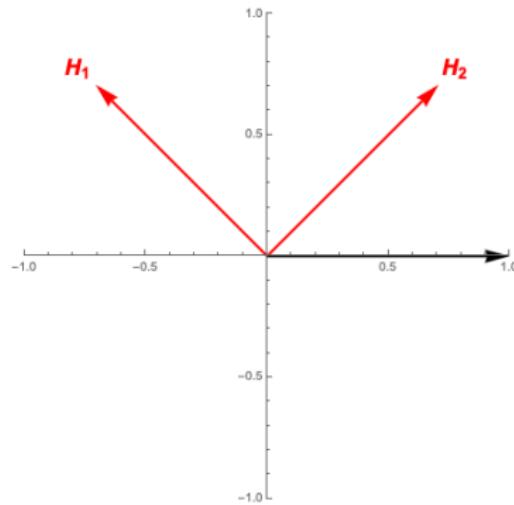
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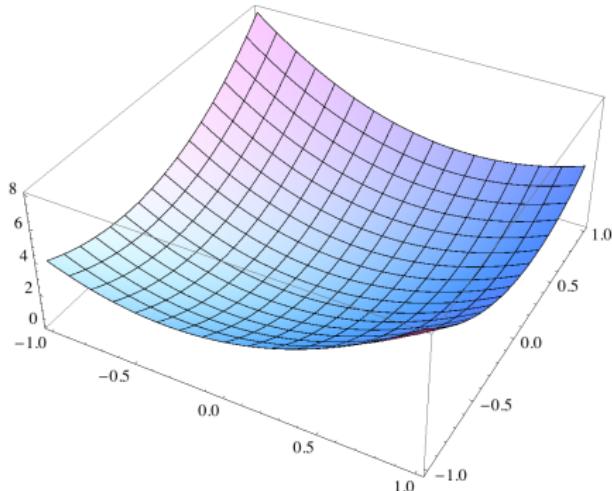
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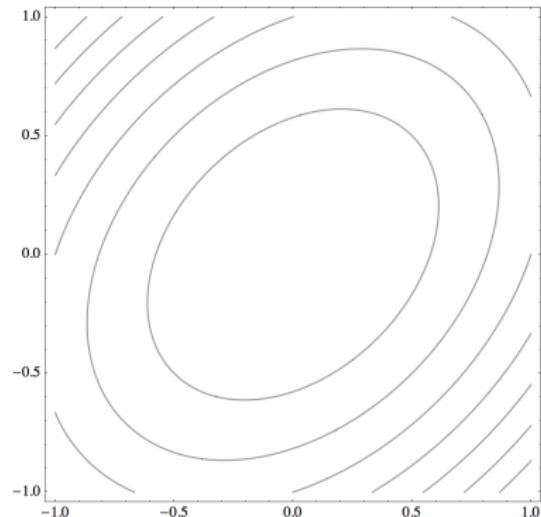
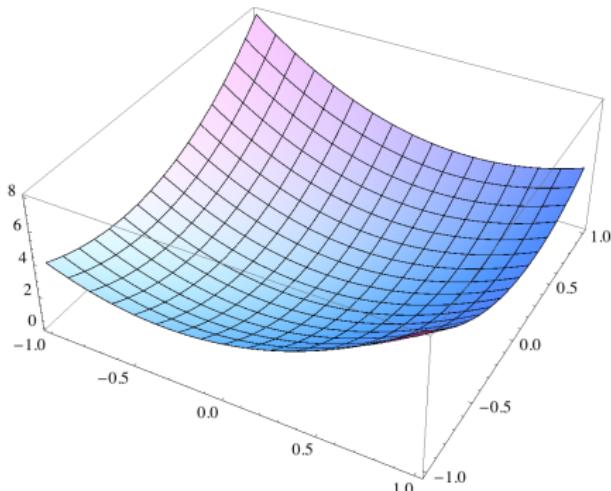
- ▶ All level sets centred in $x = 0$ by symmetry

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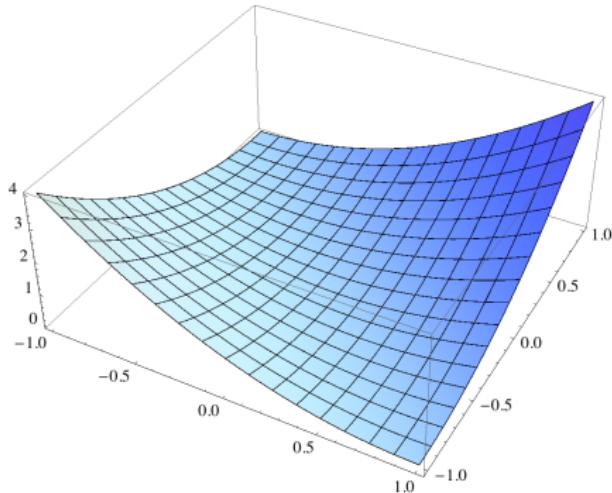
- $Q = \begin{bmatrix} 6 & -2 \\ -2 & 6 \end{bmatrix} \succ 0$ graph is a (convex) paraboloid

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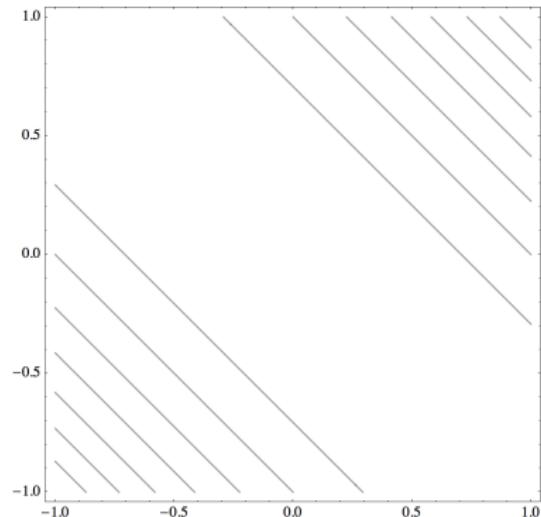
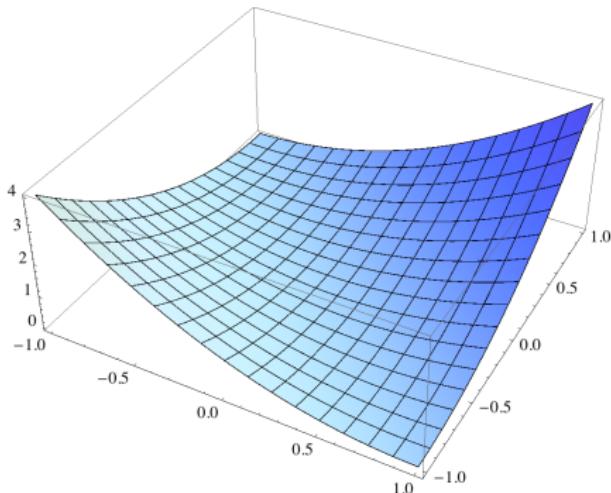
- $Q = \begin{bmatrix} 6 & -2 \\ -2 & 6 \end{bmatrix} \succ 0$ graph is a (convex) paraboloid
level sets are ellipsoids

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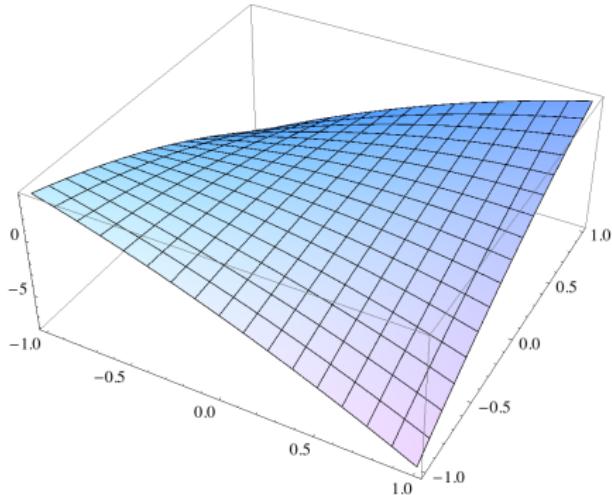
- $Q = \begin{bmatrix} 2 & 2 \\ 2 & 2 \end{bmatrix} \succeq 0$ graph is a degenerate paraboloid

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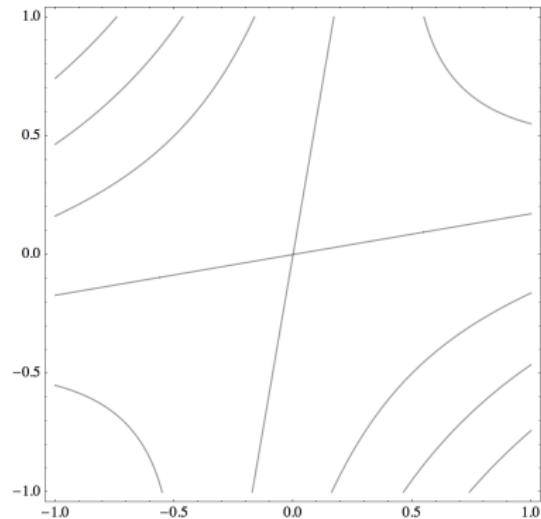
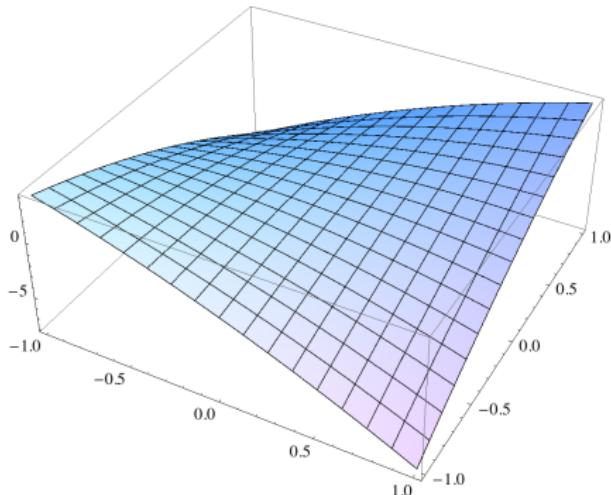
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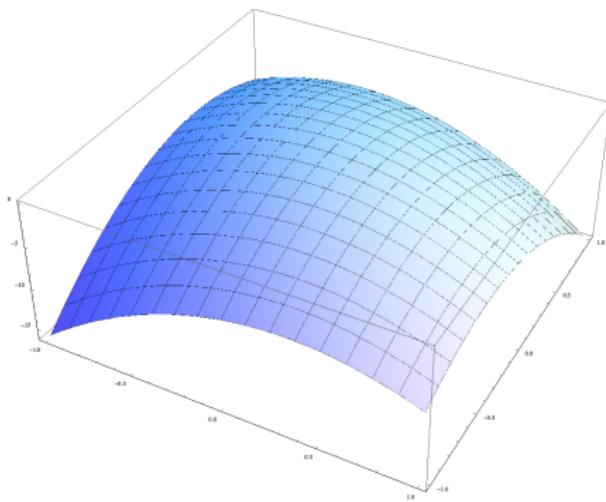
- $Q = \begin{bmatrix} 3 & -5 \\ -5 & -3 \end{bmatrix} \succcurlyeq 0$ graph saddle-shaped (0 is a saddle point)

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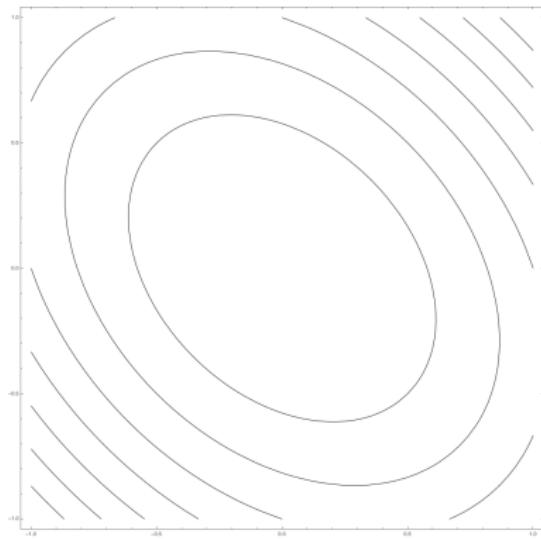
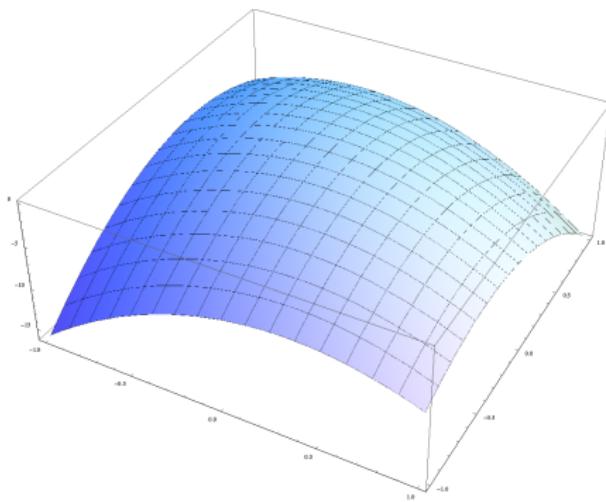
- $Q = \begin{bmatrix} 3 & -5 \\ -5 & -3 \end{bmatrix} \asymp 0$ graph saddle-shaped (0 is a saddle point)
level sets are hyperboloids

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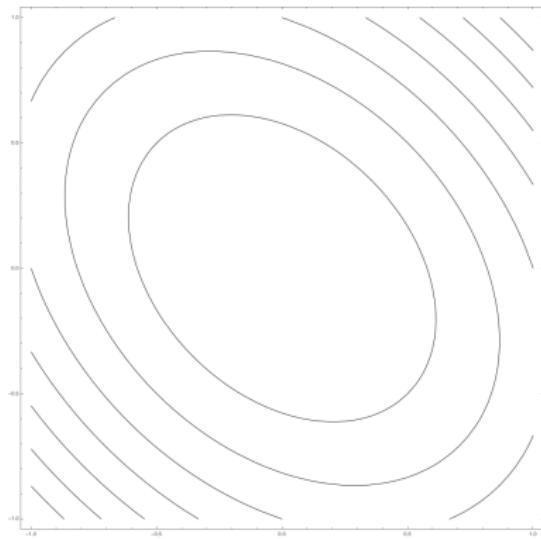
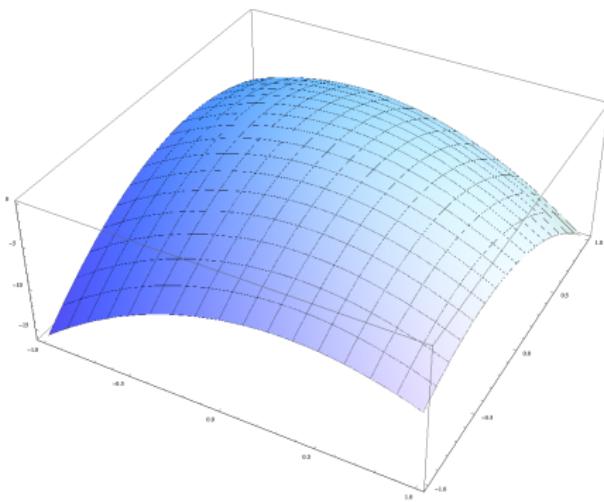
- $Q = \begin{bmatrix} -6 & -2 \\ -2 & -6 \end{bmatrix} \prec 0$ graph a (concave, i.e., “upside-down”) paraboloid

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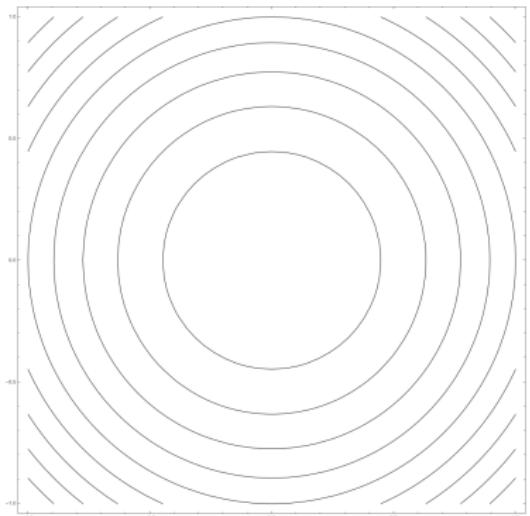


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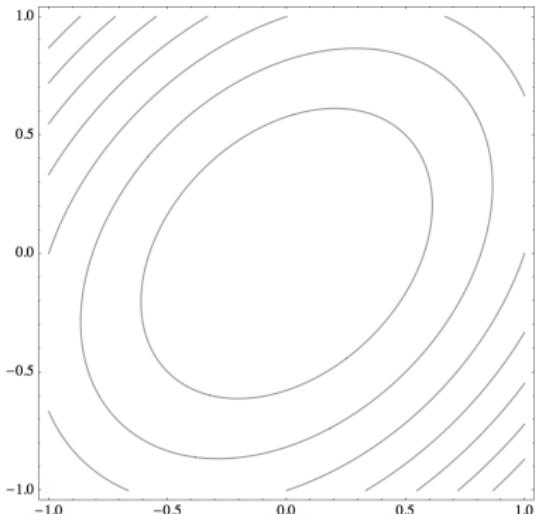


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- Level sets can be precisely described in terms of H_i, λ_i



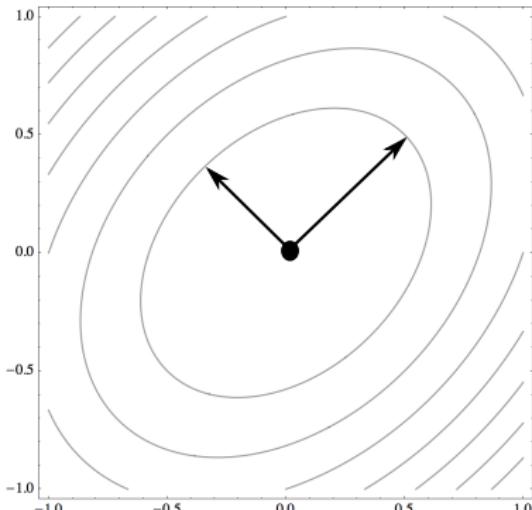
► $\|x\|_2^2 \equiv Q = H = \Lambda = I$: perfect circles

$$Q = H = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \lambda = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$



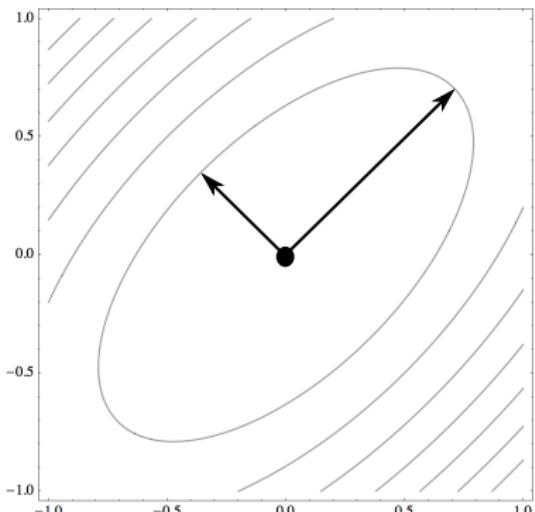
- ▶ Recall again $\varphi_{H_i}(\alpha) = \alpha^2 \lambda_i$
- ▶ $L(f, 1) \cap H_i \equiv \varphi_{H_i}(\alpha) = 1 \implies \lambda_i > 0$
- ▶ $\varphi_{H_i}(\alpha) = 1 \equiv \alpha = \sqrt{1/\lambda_i} \implies$

$$Q = \begin{bmatrix} 6 & -2 \\ -2 & 6 \end{bmatrix}, \quad H = \frac{\sqrt{2}}{2} \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}, \quad \lambda = \begin{bmatrix} 8 \\ 4 \end{bmatrix}$$



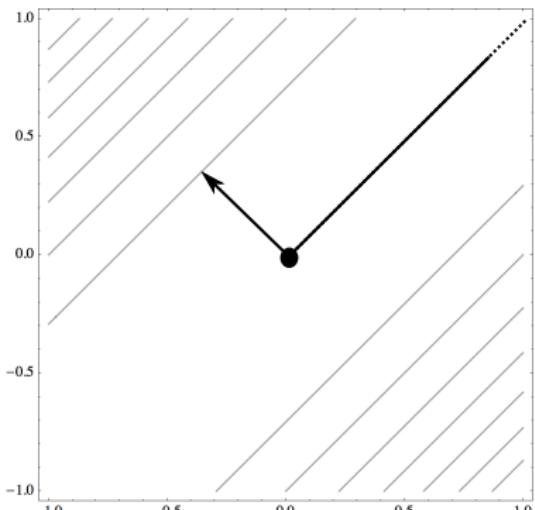
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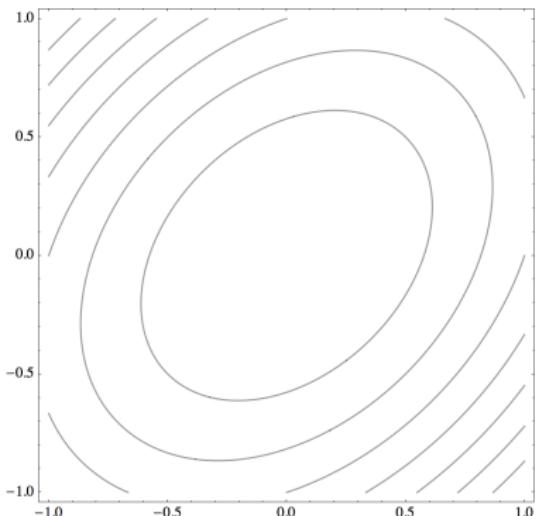
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- ▶ $\lambda_i \searrow \equiv \text{axis } \nearrow,$

$$Q = \begin{bmatrix} 5 & -3 \\ -3 & 5 \end{bmatrix}, \quad H = \frac{\sqrt{2}}{2} \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}, \quad \lambda = \begin{bmatrix} 8 \\ 2 \end{bmatrix}$$



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- ▶ $\lambda_i \searrow \equiv \text{axis } \nearrow, \lambda_i = 0 \implies \text{"axis } \rightarrow \infty\text{"}$
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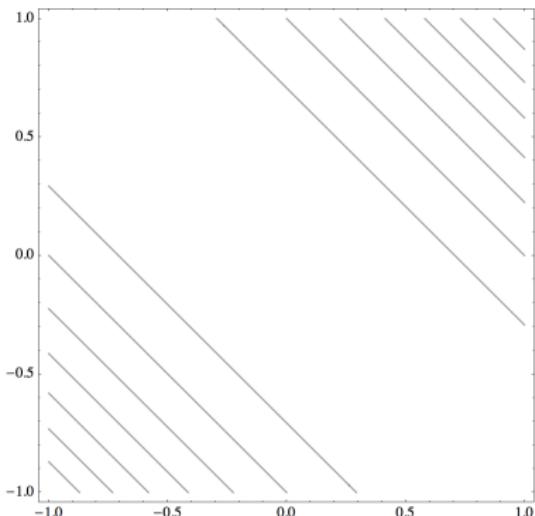
$$Q = \begin{bmatrix} 4 & -4 \\ -4 & 4 \end{bmatrix}, \quad H = \frac{\sqrt{2}}{2} \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}, \quad \lambda = \begin{bmatrix} 8 \\ 0 \end{bmatrix}$$



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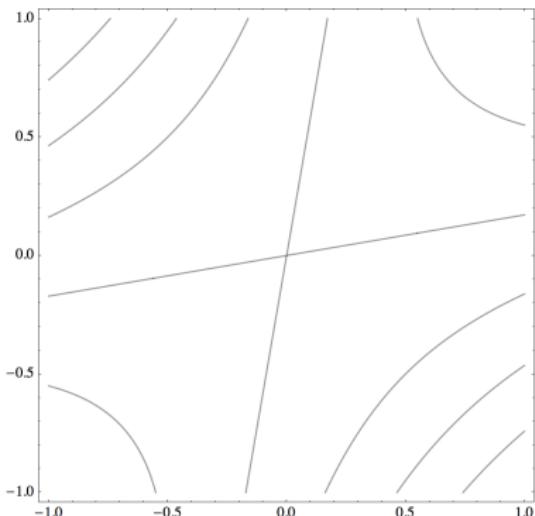
- ▶ All λ_i have the same sign: $f(x)$ either ≥ 0 or $\leq 0 \implies$ ellipsoids



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$$Q = \begin{bmatrix} 3 & -5 \\ -5 & 3 \end{bmatrix}, \quad H = \frac{\sqrt{2}}{2} \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}, \quad \lambda = \begin{bmatrix} 8 \\ -2 \end{bmatrix}$$

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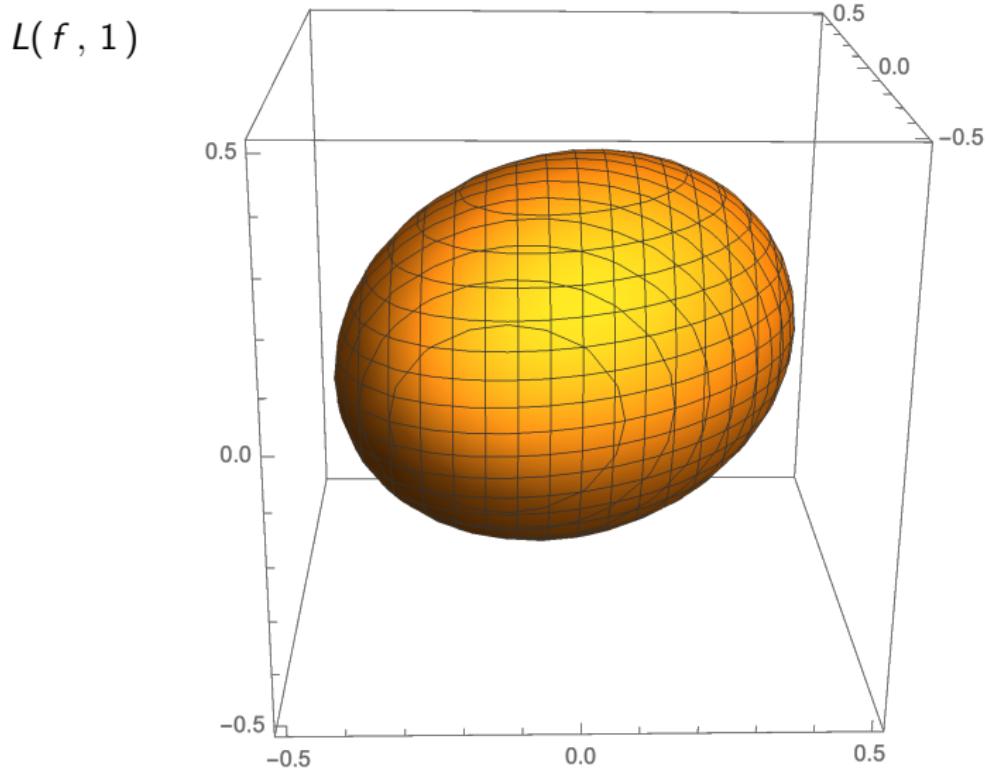
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- ▶ All λ_i have the same sign: $f(x)$ either ≥ 0 or $\leq 0 \implies$ ellipsoids
- ▶ Some $\lambda_i = 0 \implies$ "degenerate" ellipsoids (∞ axis)
- ▶ $\lambda_i > 0$ and $\lambda_j < 0$: $\exists \alpha_i, \alpha_j$ s.t. $\varphi_{H_i}(\alpha_i) + \varphi_{H_j}(\alpha_j) = 0 \implies$ hyperboloids

Level sets homogeneous quadratic functions, 3D example

37

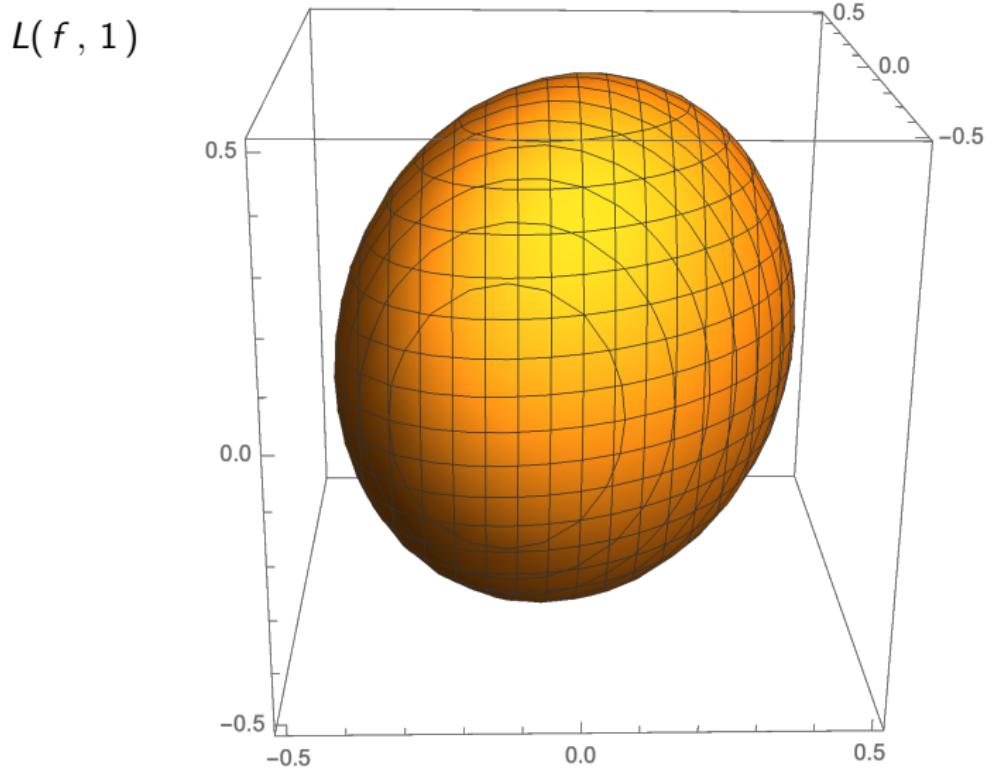
$$Q = \begin{bmatrix} 6 & -2 & 0 \\ -2 & 6 & 0 \\ 0 & 0 & 8 \end{bmatrix}, \quad H = \begin{bmatrix} -1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \lambda = \begin{bmatrix} 8 \\ 4 \\ 8 \end{bmatrix}$$



Level sets homogeneous quadratic functions, 3D example

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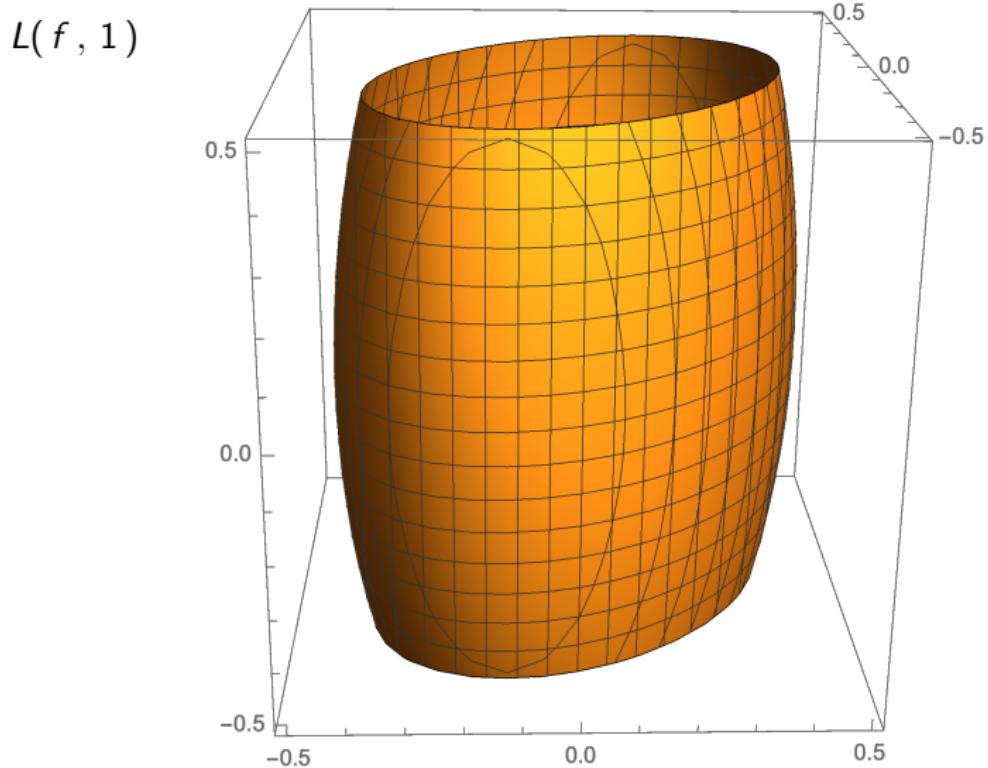
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Level sets homogeneous quadratic functions, 3D example

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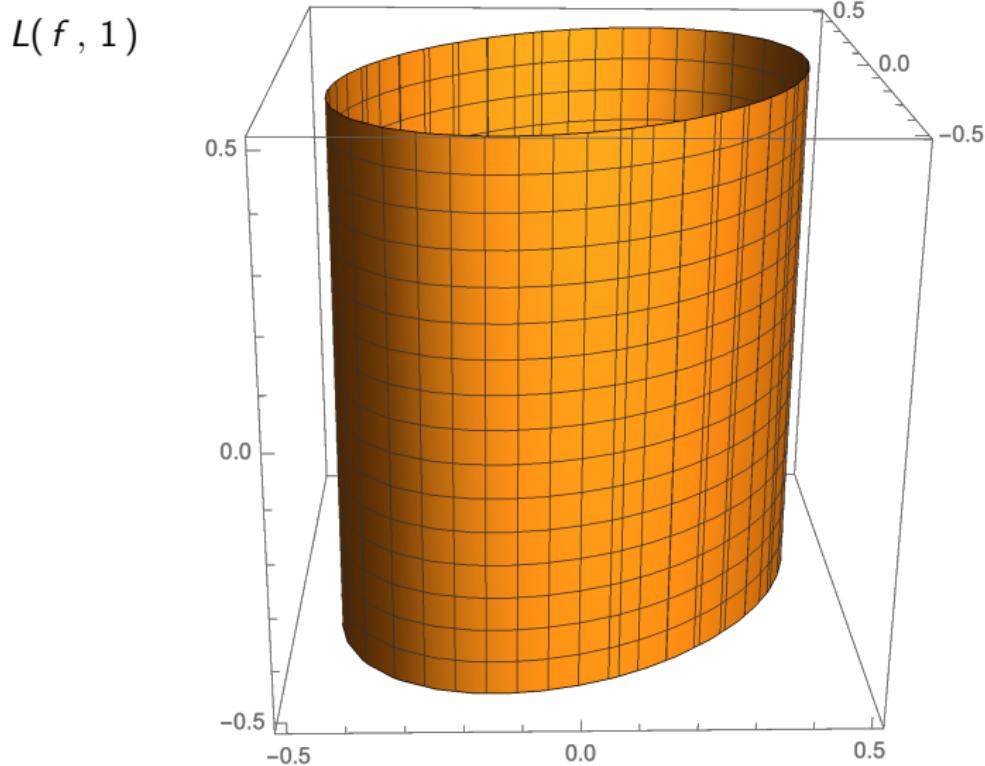
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Level sets homogeneous quadratic functions, 3D example

37

$$Q = \begin{bmatrix} 6 & -2 & 0 \\ -2 & 6 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad H = \begin{bmatrix} -1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \lambda = \begin{bmatrix} 8 \\ 4 \\ 0 \end{bmatrix}$$



► Clearly depends sign of eigenvalues of $Q \equiv$ definiteness:

- ▶ $Q \succeq 0 \wedge Q \preceq 0 \equiv \lambda_1 = \lambda_n = 0 \equiv Q = 0 \implies \min = \max = 0$ (constant)
- ▶ $Q \succeq 0 \implies \min = 0, \operatorname{argmin} = 0, \max = +\infty$
- ▶ $Q \preceq 0 \implies \max = 0, \operatorname{argmax} = 0, \min = -\infty$
- ▶ $Q \not\propto 0 \implies \max = +\infty, \min = -\infty$

analogous to univariate case, but “many more ways to be $> 0 / < 0$ ”

Exercise: Formally prove all the unboundedness results

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Exercise: Formally prove all the unboundedness results

- ▶ Box-constrained optimization on (closed) hyperrectangle X absolutely **not** analogous to the univariate case:
 - ▶ \mathcal{NP} -hard in most cases [3]
 - ▶ min with $Q \succeq 0$ and max with $Q \preceq 0$ polynomial but nontrivial (will see)
- ▶ \mathcal{NP} -hardness due to \mathbb{R}^n “big” (X has 2^n vertices), issue also in \mathcal{P} case
- ▶ $\max\{f(x)\}$ and $\min\{f(x)\}$ very very different

- $f(x) = \frac{1}{2}x^T Qx + \langle q, x \rangle$: a homogeneous quadratic plus a linear
- $q \neq 0$ but Q nonsingular $\equiv \lambda_i \neq 0 \forall i$ (regardless of the sign)
- Then $f(x) = g(z) = \frac{1}{2}z^T Qz + f(\bar{x})$ for $z = x - \bar{x}$ and $\bar{x} = -Q^{-1}q$

Exercise: Prove the result, but it should look familiar

► Optimizing a quadratic non-homogeneous function

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- ▶ $\bar{x} (\neq 0)$ centre of the level sets: repeat ► Optimizing a homogeneous quadratic multivariate function for $g(z)$, translate the results back in x -space
- ▶ Box-constrained case remains hard / nontrivial
- ▶ Analogous to univariate case, but many more ways for (pieces of) Q to be 0 and therefore the result not be applicable
- ▶ More complicated analysis needed, coming right next

- ▶ $Q \in \mathbb{R}^{n \times n}$, eigenvalue decomposition (H, Λ) , $I = \{1, 2, \dots, n\}$
- ▶ $I^0 = \{i \in I ; \lambda_i = 0\}$, $I^+ = I \setminus I^0$, both nonempty ($k = |I^0| > 0$, $h = |I^+| > 0$)
- ▶ $\ker(Q) = \{v \in \mathbb{R}^n : \exists \eta \in \mathbb{R}^k \text{ s.t. } v = \sum_{i \in I^0} \eta_i H_i\}$
- ▶ $Qv = 0 \quad \forall v \in \ker(Q) \quad [\supset \{0\}] \quad (\text{check})$
- ▶ $\text{im}(Q) = \{w \in \mathbb{R}^n : \exists \mu \in \mathbb{R}^h \text{ s.t. } w = \sum_{i \in I^+} \mu_i H_i\}$:
- ▶ $\forall w \in \text{im}(Q) \exists x \in \mathbb{R}^n \text{ s.t. } Qx = w, \text{im}(Q) = \text{im}(-Q)$

Exercise: Prove the result (recall $Q = \lambda_1 H_1 H_1^T + \dots + \lambda_n H_n H_n^T$, use [16])

- ▶ $\mathbb{R}^n = \text{im}(Q) + \ker(Q)$, $\text{im}(Q) \perp \ker(Q)$ (H is a hortonormal base of \mathbb{R}^n)
- ▶ $q = q^+ + q^0$, $q^+ \perp q^0$, with $q^0 \in \ker(Q) \equiv Qq^0 = 0$, and
 $q^+ \in \text{im}(Q) = \text{im}(-Q) \equiv \exists \bar{x} \text{ s.t. } (-Q)\bar{x} = q^+$
- ▶ Then $f(x) = g(z) = \frac{1}{2}z^T Q z + \color{red}q^0 z + f(\bar{x})$ for $z = x - \bar{x}$

Exercise: Prove the result, but it should look very very familiar

- ▶ f is “truly quadratic” on $\text{im}(Q)$ but actually linear on $\ker(Q)$
- ▶ No surprise: $v \in \ker(Q) \implies f(v) = qv$
- ▶ Assume $Q \succeq 0$: f has minimum $\iff q^0 = 0 \equiv Q\bar{x} = -q$ has solution $\equiv q \in \text{im}(Q)$
- ▶ \bar{x} is not unique, in fact ∞ -ly many of them: “all are centres”
- ▶ \bar{x} solution $\implies \bar{x} + v$ solution $\forall v \in \ker(Q)$, all have the same objective value \equiv they are all and only the minima of f

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- ▶ Box-constrained version \mathcal{P} (but nontrivial) if $Q \succeq 0 / Q \preceq 0$, hard otherwise

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- ▶ All in all: solving system $Q\bar{x} = -q$ (or proving no solutions) required

Outline

Optimization Problems

Optimization is difficult

Simple Functions, Univariate case

Simple Functions, Multivariate case

Multivariate Quadratic case: Gradient Method

Wrap up & References

Solutions

- ▶ If one is lucky, optimising a quadratic function \equiv solving $Q\bar{x} = -q$
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- ▶ Linear system $O(n^3)$ at worst, so **not doable** for $n \approx 10^{9+}$ (no memory)
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 \implies a **sequence $\{x^i\}$** that should “go towards an optimal solution”
- ▶ The natural way: $\{f^i = f(x^i)\}$ sequence of values “go towards f_* ”
- ▶ Typically we **can't get f_* in finite time** ($\exists i \ v_i = f_*$), but we can
“get as close as we want”: **there in the limit**
- ▶ Recall: (infinite) sequence $\{v_i\} = \{v_1, v_2, \dots\}$,
 $\{v_i\} \rightarrow v \equiv \lim_{i \rightarrow \infty} v_i = v \equiv \forall \varepsilon > 0 \ \exists h \text{ s.t. } |v_i - v| \leq \varepsilon \ \forall i \geq h$
 $\lim_{i \rightarrow \infty} v_i = +\infty \iff \forall M > 0 \ \exists h \text{ s.t. } v_i \geq M \ \forall i \geq h$

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- ▶ $\{x^i\}$ s.t. $\{f^i\} \rightarrow f_*$ a **minimizing sequence**
- ▶ note that $\{f^i\} \rightarrow -\infty \implies f_* = -\infty \implies$ minimizing sequence
- ▶ A sequence **may not have limit**: are we “not converging”?
- ▶ Any monotone sequence has a **limit** (monotone algorithms are good)

- ▶ We generally assume minimization, but maximization is equivalent
- ▶ Given x^i , necessarily compute $g^i = Qx^i + q$: if $g^i = 0$ then stop
- ▶ “ $g^i = 0$ ” not doable in floating point arithmetic $\implies \|g^i\| \leq \varepsilon$ (which ε ?)
- ▶ Idea: if $\|g^i\| > [\varepsilon >] 0$, produce a x^{i+1} “better” than x^i
- ▶ How? Consider the tomography $\varphi_{x^i, -g^i}(\alpha) = f(x^i - \alpha g^i) - f(x^i)$
 $= \frac{1}{2}(x^i - \alpha g^i)^T Q(x^i - \alpha g^i) + q(x^i - \alpha g^i) - f(x^i)$
 $= \frac{1}{2}\alpha^2(g^i)^T Qg^i - \alpha[(g^i)^T Qx^i + qg^i] = \frac{1}{2}\alpha^2(g^i)^T Qg^i - \alpha\|g^i\|^2$
positive negative
- ▶ For some $\alpha > 0$, $\varphi_{x^i, -g^i}(\alpha) < 0 \implies f(x^i - \alpha g^i) < f(x^i)$

Exercise: Check all the above (recall [Optimizing a quadratic non-homogeneous function](#))

- ▶ The same information (called gradient, we'll see why) saying “you can't stop” is at the same time saying “you can get a better solution than x^i over there”
- ▶ This immediately suggests a (monotone, $f^{i+1} < f^i$) algorithm

- ▶ In fact it is easy to minimize $\varphi_{x^i, -g^i}(\alpha)$ (Optimizing a quadratic non-homogeneous function)
 $\alpha^i = \|g^i\|^2 / ((g^i)^T Q g^i) \quad [1/\lambda_1 \leq \alpha \leq 1/\lambda_n \text{ (check)}]$
- ▶ Computing g^i and the optimal value of α is $O(n^2)$ \Rightarrow
 n "large" \Rightarrow "we can do many iterations before hitting $O(n^3)$ "

```

procedure  $x = SDQ(Q, q, x, \varepsilon)$ 
do forever
     $g \leftarrow Qx + q;$ 
    if(  $\|g\| \leq \varepsilon$  ) then break;
     $\alpha \leftarrow \text{stepsize}(); x \leftarrow x - \alpha g;$ 

```

- ▶ stepsize() { return($\|g\|^2 / (g^T Q g)$); }, others possible

Exercise: something can go wrong with that formula \uparrow : what does it mean?
 Improve the pseudo-code to take that occurrence into account.

Exercise: what happens if $Q \not\succeq 0$? Does the (improved) code need be fixed?

Exercise: Discuss how to change the code to solve $\max\{f(x)\}$ instead

Exercise: Rewrite the code with one product with Q per iteration

- ▶ It is very simple, but does it work? And is it efficient?

- Optimal stepsize $\implies g^{i+1} \perp g^i$ (**check**)
- “Homogeneous form of the error”: $A(x) = \frac{1}{2}(x - x_*)^T Q(x - x_*)$ (**check**)
- The above for $x = x^{i+1}$, $Q \succ 0$ and some algebra [5, Lm. 8.6.1] gives

$$A(x^{i+1}) = \left(1 - \frac{\|g^i\|^4}{((g^i)^T Q g^i)((g^i)^T Q^{-1} g^i)} \right) A(x^i) \quad (\text{check}) [\text{tedious}]$$

- Easy to derive an estimate using $\kappa = \lambda_1 / \lambda_n$ [≥ 1] condition number of Q

$$\frac{\|x\|^4}{(x^T Q x)(x^T Q^{-1} x)} \geq \frac{\lambda_n}{\lambda_1} = \frac{1}{\kappa} \quad (\text{check}) \implies A(x^{i+1}) \leq \left(1 - \frac{1}{\kappa} \right) A(x^i)$$

- This means the algorithm **converges**: $A(x^i) \leq r^i A(x^0)$ (**check**) with $r \leq (\kappa - 1) / \kappa < 1 \implies A(x^i) \rightarrow 0$ **exponentially fast** as $i \rightarrow \infty$

- Kantorovich inequality [5, 8.6.(34)] gives better estimate

$$\frac{\|x\|^4}{(x^T Q x)(x^T Q^{-1} x)} \geq \frac{4\lambda_1\lambda_n}{(\lambda_1 + \lambda_n)^2} \implies r \leq \left(\frac{\lambda_1 - \lambda_n}{\lambda_1 + \lambda_n} \right)^2 = \left(\frac{\kappa - 1}{\kappa + 1} \right)^2$$

- Let's see it in practice

- Crucial sequences: $\{x^i\} / \{d^i = \|x^i - x_*\|\}$ [iterates / distance from x_*]
 $\{f^i = f(x^i)\} / \{a^i = A(x^i)\} / \{r^i = R(x^i)\}$ [f -values / A/R gaps]
- Complexity as a function of prescribed accuracy ε :
 max number of iterations k such that $d^i / a^i / r^i \leq \varepsilon \forall i \geq k$
- General formula: $v^k \leq r^k v^1 \leq \varepsilon$ for $k \geq [1 / \log(1/r)] \log(v^1 / \varepsilon)$ (check)
- $r \approx 1 \implies k \in O([r/(1-r)] \log(v^1 / \varepsilon))$ (check)
- Good news: dimension independent (n not there) \implies very-large-scale
- $O(\log(1/\varepsilon))$ (good), but the constant $\uparrow \infty$ as $r \rightarrow 1$ (bad)
- $v^1 = f(x^1) - f_*$: starting closer to f_* helps (would be strange if not)
- " $\|x^i - x_*\| \leq \varepsilon$ " and " $f(x^i) - f_* \leq \varepsilon$ " not the same (ε):
 $a^i = \frac{1}{2}(x^i - x_*)^T Q(x^i - x_*) \leq \varepsilon \implies \lambda_n \|x^i - x_*\|^2 \leq \varepsilon \implies$
 $d^i = \|x^i - x_*\| \leq \sqrt{\varepsilon / \lambda_n}$

Exercise: Cook up the other direction ($d^i \leq \varepsilon \implies \dots$)

- Converge: $\{f^i\} \rightarrow f_* \approx \{a^i\} \rightarrow 0 \equiv \{r^i\} \rightarrow 0 \Leftarrow \{d^i\} \rightarrow 0$ ($\not\Rightarrow$)

Exercise: Discuss why $\{f^i\} \rightarrow f_*$ is only \approx to $\{a^i\} \rightarrow 0$ and why the $\not\Rightarrow$

- But how rapidly does it ("in the tail")? Rate/order of convergence

$$\lim_{i \rightarrow \infty} \left[\frac{f^{i+1} - f_*}{(f^i - f_*)^p} = \frac{a^{i+1}}{(a^i)^p} \approx \frac{r^{i+1}}{(r^i)^p} \right] = r \quad \begin{cases} x^p \rightarrow 0 \text{ faster than } x \rightarrow 0 \text{ when } p > 1 \\ x \rightarrow 0 \text{ when } p < 1 \end{cases} \quad (\text{check})$$

- $p = 1, r = 1 \equiv$ sublinear: important examples

error $O(1/i)$	$O(1/i^2)$	$O(1/\sqrt{i})$
i	$O(1/\varepsilon)$ (bad)	$O(1/\sqrt{\varepsilon})$ (a bit better)
		$O(1/\varepsilon^2)$ (horrible)

- $p = 1, r < 1 \equiv$ linear: $r^i \implies i \in O(\log(1/\varepsilon))$ (good unless $r \approx 1$)

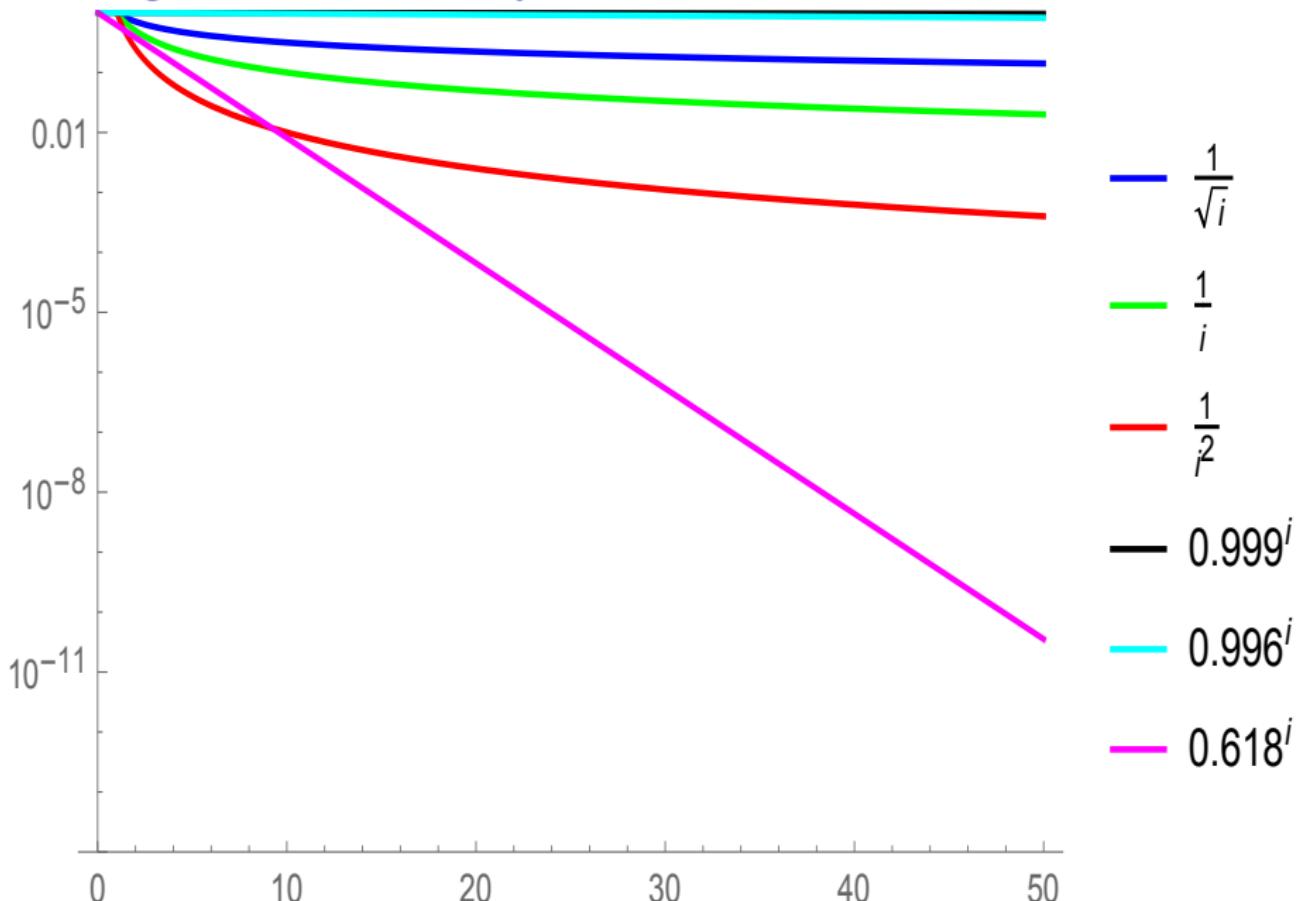
- $p = 2, r > 0 \equiv$ quadratic (!!): $\approx 1/2^{2^i} \implies i \in O(\log(\log(1/\varepsilon)))$
in practice $O(1)$ (correct digits double at each iteration)

- $p \in (1, 2) \equiv p = 1, r = 0 \equiv$ superlinear (!): "something in the middle"

- $p = 2$ the best you can reasonably hope for: possible but not easy

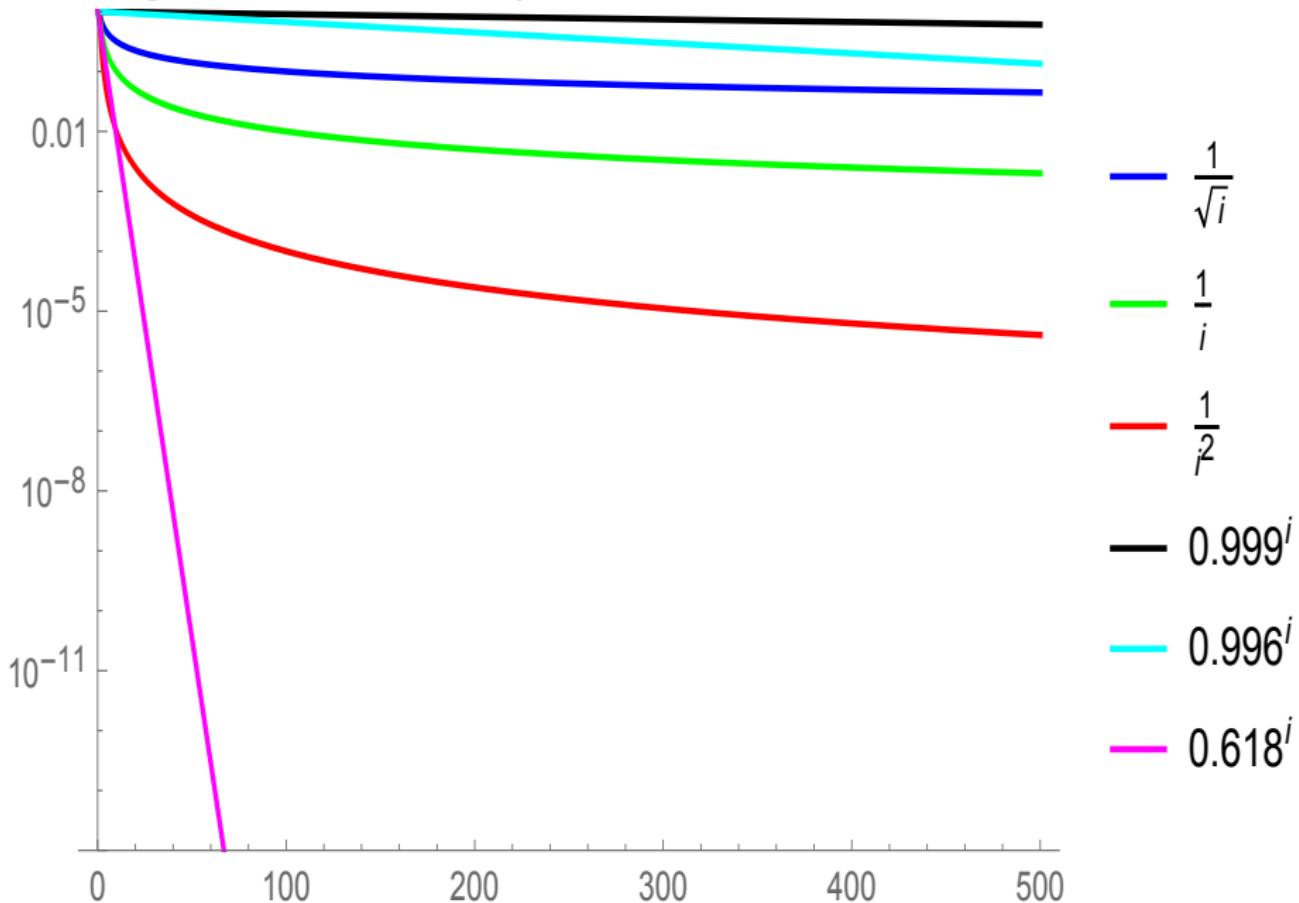
Convergence Rates Pictorially

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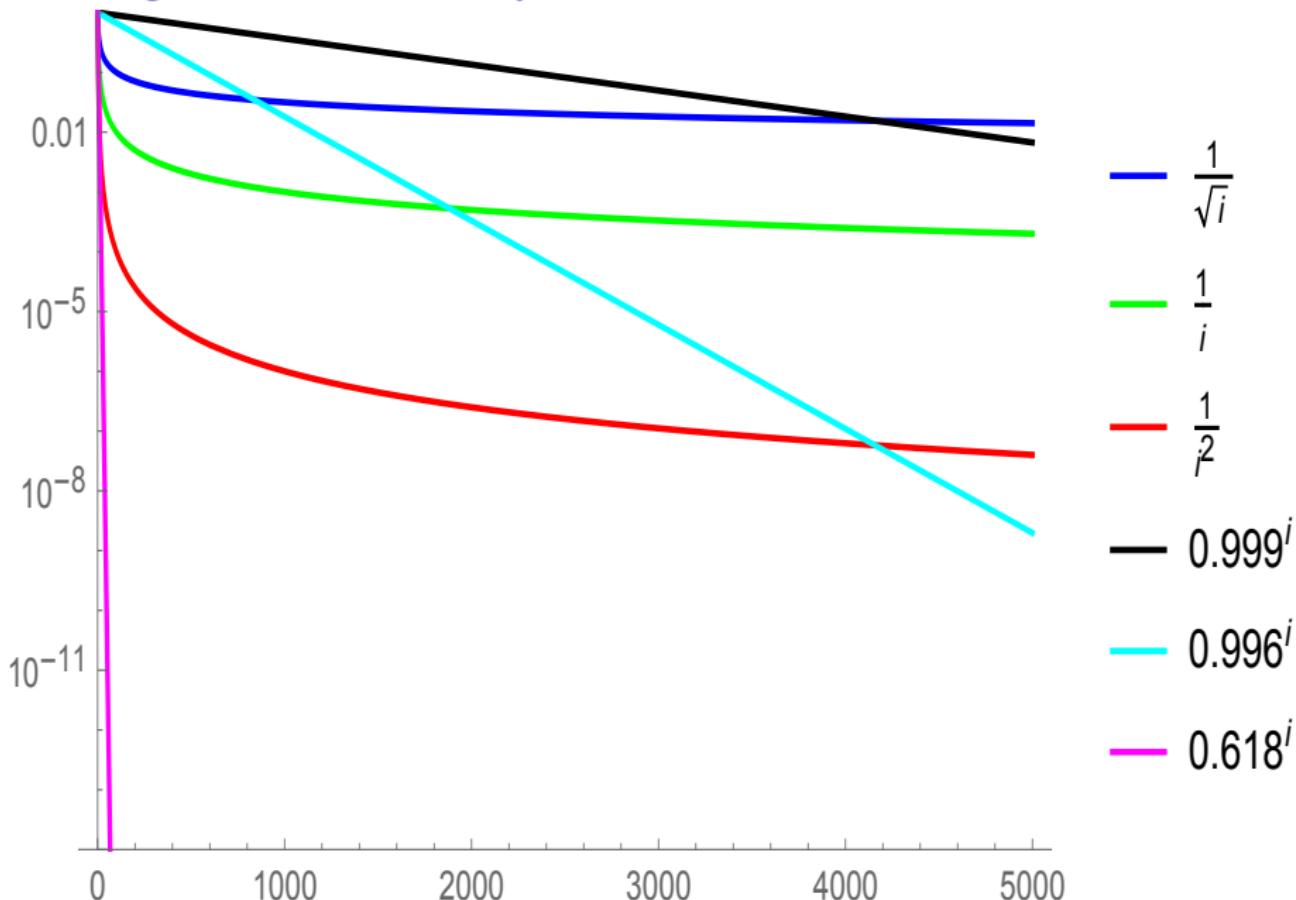
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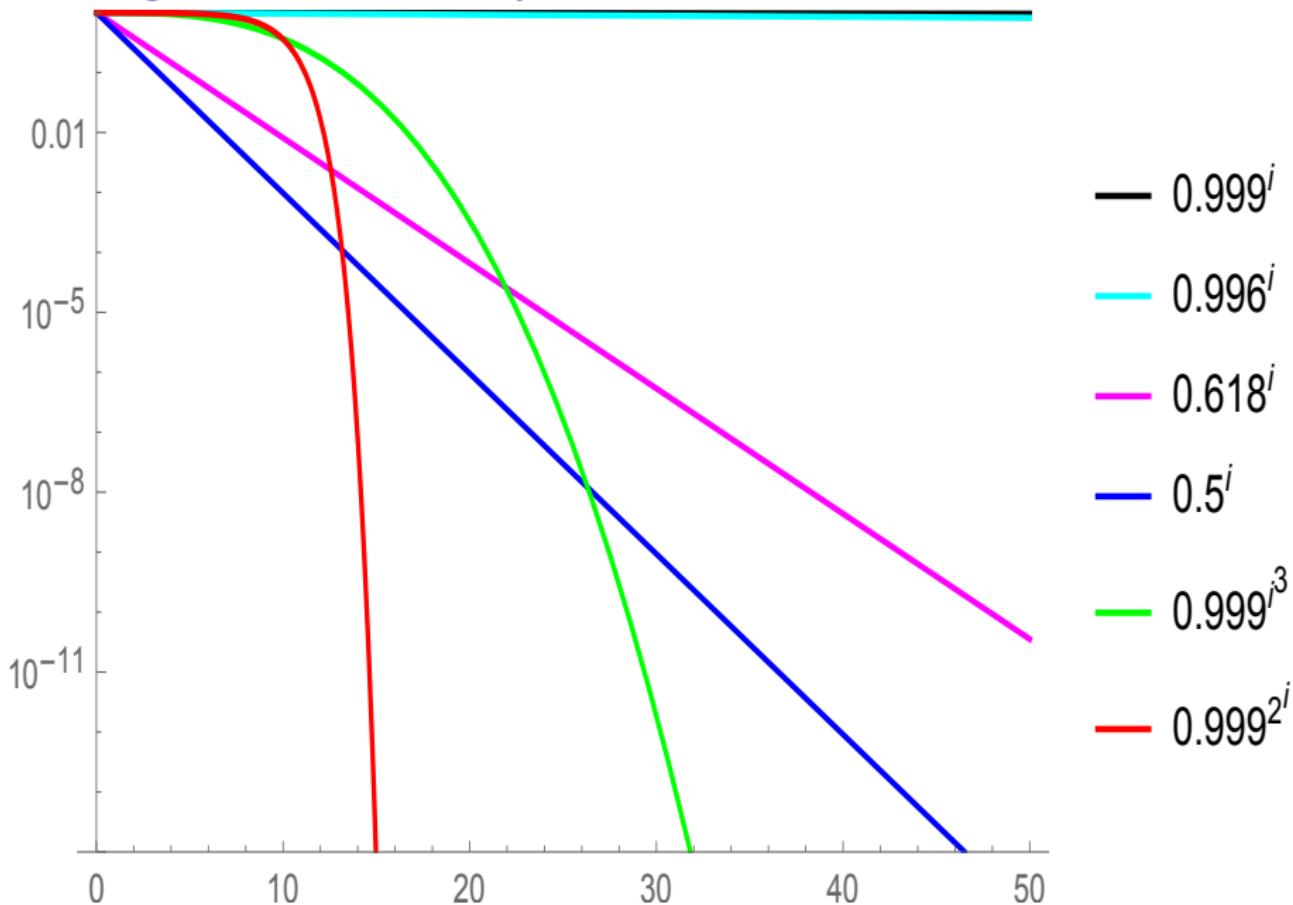
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- ▶ The stopping criterion one **would want**: $A(x^i) \leq \varepsilon$ / $R(x^i) \leq \varepsilon$
- ▶ Issue: f_* typically unknown, cannot be used on-line
- ▶ $\|g^i\|$ "proxy" of $A(x^i)$: hopefully $\|g^i\|$ "small" $\implies A(x^i)$ "small"
but exact relationship nontrivial \implies choosing ε non obvious
- ▶ $\|g^i\| = Q(x^i - x_*) \implies \|g^i\| \leq \lambda_1 \|x^i - x_*\| \dots$ (??) wrong inequality:
 $\|g^i\| \leq \varepsilon \not\implies \|x^i - x_*\|$ "small"
- ▶ $a^i = \frac{1}{2}(x^i - x_*)^T Q(x^i - x_*) = \frac{1}{2} \langle x^i - x_*, g^i \rangle \leq \frac{1}{2} \|g^i\| \|x^i - x_*\|$;
if we knew $\delta \geq \|x^i - x_*\|$, which we don't, then $\|g^i\| \leq 2\varepsilon / \delta \implies a^i \leq \varepsilon$
- ▶ If we knew $\lambda_n > 0$, which we don't, $\|g^i\| \leq \sqrt{2\lambda_n \varepsilon} \implies a^i \leq \varepsilon$ (**check**)
- ▶ All in all, exact control on final a^i / r^i not obvious (not always really needed)

- ▶ Convergence **fast** if $\lambda_1 \approx \lambda_n$ (one iteration for $\|x\|^2$), **rather slow** if $\lambda_1 \gg \lambda_n$:
 $\kappa = \lambda_1 / \lambda_n \rightarrow \infty$ (Q ill conditioned) $\implies r \rightarrow 1 \implies$ slow in practice
- ▶ $g^{i+1} \perp g^i$ + level sets very elongated \implies lots of “zig-zags” \implies slow
- ▶ Ex.: $\kappa = 1000 \implies r \approx 0.996 \implies r/(1-r) \approx 250$
 $f(x^1) - f_* = 1, \varepsilon = 10^{-6} \implies k \geq 3450$ for $n = 2$

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 $f(x^1) - f_* = 1, \varepsilon = 10^{-6} \implies k \geq 3450$ for $n = 2 \dots$ but also for $n = 10^8$
- ▶ Note: with coarser formula $r = 0.999 \equiv r / (1 - r) \approx 1000 \implies k \geq 13800$
- ▶ In other words: $0.996^{10} \approx 0.96071$ $0.999^{10} \approx 0.99004$

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- ▶ Note: with coarser formula $r = 0.999 \equiv r / (1 - r) \approx 1000 \implies k \geq 13800$
- ▶ In other words: $0.996^{2000} \approx 0.00033$ $0.999^{2000} \approx 0.13520$

- ▶ Convergence **fast** if $\lambda_1 \approx \lambda_n$ (one iteration for $\|x\|^2$), **rather slow** if $\lambda_1 \gg \lambda_n$:
 $\kappa = \lambda_1 / \lambda_n \rightarrow \infty$ (Q ill conditioned) $\implies r \rightarrow 1 \implies$ slow in practice
- ▶ $g^{i+1} \perp g^i$ + level sets very elongated \implies lots of “zig-zags” \implies slow
- ▶ Ex.: $\kappa = 1000 \implies r \approx 0.996 \implies r / (1 - r) \approx 250$
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- ▶ In other words: $0.996^{2000} \approx 0.00033$ $0.999^{2000} \approx 0.13520$
- ▶ More bad news, “hidden dependency”:
 λ_1 and λ_n may depend on n , κ may grow as $n \rightarrow \infty$
- ▶ More bad news: the behaviour in practice is close to the bound
- ▶ Even more bad news: $\lambda_n = 0 \equiv \kappa = \infty$ happens

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- ▶ $\lambda_n = 0 \implies$ not converging? No, just can't prove it this way
- ▶ In fact we can prove convergence (in a more general setting) [2, Theorem 3.3]:
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- ▶ Is it good news? Only partly. Because complexity is $k \geq 2\lambda_1 d^1 / \varepsilon$
- ▶ $O(1/\varepsilon)$ vs. $O(\log(1/\varepsilon))$: sublinear convergence, exponentially slower
- ▶ One further digit of accuracy \equiv 10 times more iterations \implies typically unfeasible to get more than $1e-3 / 1e-4$ accuracy
- ▶ The result cannot be improved (in general, will see)
- ▶ Is it bad? Rather. Can it be worse? Yes (in general, will see)

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- ▶ Is it bad? Rather. Can it be worse? Yes (in general, will see)
- ▶ If $\lambda_n > 0$, can we do better than $O(\log(1/\varepsilon))$? Yes – @Federico
- ▶ Fundamental idea, will see more than once: changing the space

Outline

Optimization Problems

Optimization is difficult

Simple Functions, Univariate case

Simple Functions, Multivariate case

Multivariate Quadratic case: Gradient Method

Wrap up & References

Solutions

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- ▶ Solving (simple) optimization problems requires linear algebra, and vice-versa
- ▶ We now know all we need about simple problems, time to step up the game
- ▶ Will keep following an incremental approach: next step is more complicated functions but only one variable

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- ▶ Use $\max\{ |f_*|, 1 \}$ instead; this corresponds to $\min\{ f(x) + 1 \}$ [back]
- ▶ $b > 0$ and $x - z > 0 \implies b(x - z) > 0 \equiv bx > bz$;
the others are analogous (or simpler) [back]
- ▶ If $x_+ = +\infty$, obviously $x_* = +\infty = x_+$
If $x_+ < +\infty$, since $f(x)$ is increasing, $f(x) < f(x_+) \forall x < x_+$
The treatment of x_- is analogous.
If $b < 0$, the role of x_+ and x_- reverses ($x_+ = \text{argmin}$, $x_- = \text{argmax}$)
If $b = 0$, every point in X is an optimal solution [back]
- ▶ $x > z$, $a > 0$ and $x > 0 \implies ax^2 > axz > az^2$. Since $f(x)$ is symmetric ($ax^2 = a(-x)^2$), increasing for $x > 0 \equiv$ decreasing for $x < 0$. When $a < 0$ the sign of the inequalities is inverted (the function is reflected upon the x axis).
The case $a = 0$ is trivial [back]

- ▶ $f(x)$ has a minimum in 0, is decreasing for $x < 0$ and increasing for $x > 0$. If $x_- > 0$ then $f(x)$ is increasing along all X , hence x_- is the minimum and x_+ the maximum. The argument is symmetric if $x_+ < 0$. Obviously, if $0 \in X$ then it is the minimum; for the maximization, since the function is increasing when x moves away from 0 in both directions, the maximum has to be one of the two extremes but we don't know which until we test. The rest is too trivial [back]
- ▶ No, this is both too trivial and didactic [back]
- ▶ $f(x) = (ax + b)x$, hence the roots are $x = 0$ and $x = x_p = -b/a$. Clearly, $\bar{x} = -b/2a$ is always in the middle of the interval defined by the roots. If a and b have the same sign then $x_p < \bar{x} < 0$, otherwise $x_p > \bar{x} > 0$ [back]
- ▶ $\varphi_{x,(\beta d)}(\alpha) = f(x + \alpha(\beta d)) = f(x + (\alpha\beta)d) = \varphi_{x,d}(\alpha\beta)$ [back]

- ▶ We assume that i. and ii. hold for f and we want to show that $f(x) = \langle b, x \rangle$ for some $b \in \mathbb{R}^n$. Let $u_i, i = 1, \dots, n$, the i -th vector of the canonical base of \mathbb{R}^n (having 1 in the i -th position and 0 otherwise), and $b_i = f(u_i)$. For any $x \in \mathbb{R}^n$, $x = \sum_{i=1}^n x_i u_i$, hence $f(x) = f(\sum_{i=1}^n x_i u_i) = \sum_{i=1}^n f(x_i u_i)$ (using ii. recursively n times) $= \sum_{i=1}^n x_i f(u_i)$ (using i. on each individual term) $= \sum_{i=1}^n b_i x_i$ (using the definition of b_i) $= \langle b, x \rangle$ (using the definition of scalar product). The results clearly breaks in the affine case ($c \neq 0$):
$$f(x) = x + 1 \implies f(2x) = 2x + 1 \neq 2(x + 1) = 2f(x) \quad [\text{back}]$$
- ▶ By contradiction, $\exists \gamma \in \mathbb{R}^n \setminus \{0\}$ s.t. $H\gamma = 0 \implies 0 = \|H\gamma\|^2 = \gamma^T [H^T H]\gamma = \|\gamma\|^2 > 0 [\gamma \neq 0] \quad \notin \quad [\text{back}]$

- ▶ This is based on a general result: for $[A^1, A^2, \dots, A^n] = A \in \mathbb{R}^{m \times n}$ (not necessarily square) written by columns, $AA^T = M \in \mathbb{R}^{m \times m}$ (symmetric, prove it using $[AB]^T = B^T A^T$) can be written as the sum of the n rank-one matrices corresponding to the columns, i.e., $M = \sum_{i=1}^n [D^i = A^i(A^i)^T]$. In fact, the h -th row of A is $A_h = [A_h^1, A_h^2, \dots, A_h^n]$ and the k -th column of A^T is the k -th row of A , thus $M_{hk} = \langle A_h, A_k \rangle = \sum_{i=1}^n A_h^i A_k^i$. But $D_{hk}^i = A_h^i A_h^i$, hence $M_{hk} = \sum_{i=1}^n D_{hk}^i$ for all h and k
 To complete the result, for $\Lambda = \text{diag}([\lambda_1, \lambda_2, \dots, \lambda_n]) \in \mathbb{R}^{n \times n}$, $L = A\Lambda = [\lambda_1 A^1, \lambda_2 A^2, \dots, \lambda_n A^n]$. In fact, the h -th row $A_h = [A_h^1, A_h^2, \dots, A_h^n]$ and the k -th column of Λ , i.e., $\lambda_k u_k$ (u_k being the k -th vector of the canonical base) give $L_{hk} = \langle A^h, \lambda_k u_k \rangle = \lambda_k A_h^k$ **[back]**
- ▶ $\varphi_{H_i}(\alpha) = (\alpha H_i)^T Q(\alpha H_i) = \alpha^2 [H_i^T (\lambda_i H_i)] = \lambda_i \alpha^2$ **[back]**
- ▶ $\lambda_n < 0 \implies \varphi_{H_n}(\alpha) [= \lambda_n \alpha^2]$ unbounded below $\implies f(x)$ unbounded below
 $\lambda_1 > 0 \implies \varphi_{H_1}(\alpha)$ unbounded above $\implies f(x)$ unbounded above **[back]**

- ▶ $x = z + \bar{x} \implies \frac{1}{2}x^T Qx + qx = \frac{1}{2}(z + \bar{x})^T Q(z + \bar{x}) + q(z + \bar{x}) = \frac{1}{2}z^T Qz + z^T(Q\bar{x} + q) + [\frac{1}{2}\bar{x}^T Q\bar{x} + q\bar{x}] = \frac{1}{2}z^T Qz + f(\bar{x})$
as $Q\bar{x} + q = Q(-Q^{-1}q) + q = -q + q = 0$ [back]
- ▶ $Qv = Q[\sum_{i \in Z} \eta_i H_i] = \sum_{i \in Z} \eta_i QH_i = \sum_{i \in Z} \eta_i \lambda_i H_i = 0$ [back]
- ▶ $Q = H\Lambda H^T = \sum_{i=1}^n \lambda_i H_i H_i^T = \sum_{i \in Z} \lambda_i H_i H_i^T [= 0] + \sum_{i \in N} \lambda_i H_i H_i^T$
We want to prove $\exists x$ s.t. $(\sum_{i \in N} \lambda_i H_i H_i^T)x = \sum_{i \in N} \mu_i H_i = w$
True if $\lambda_i H_i^T x = \mu_i$ $i \in N \equiv H_i^T x = \gamma_i = \mu_i / \lambda_i$ $i \in N$,
a linear system of $k \leq n$ equations in n variables (likely underdetermined)
All H_i linearly independent, $H_N = [H_i]_{i \in N} \in \mathbb{R}^{n \times k} \implies \text{rank}(H_N) = k$
 $\implies [H_N^T, \gamma] \in \mathbb{R}^{k \times n+1}$ has rank k (rank \leq number of rows) \implies
by [16] the system has a solution x (∞ -ly many if $k < n$) [back]
- ▶ $\frac{1}{2}x^T Qx + qx = \frac{1}{2}(z + \bar{x})^T Q(z + \bar{x}) + q(z + \bar{x}) = \frac{1}{2}z^T Qz + z^T(Q\bar{x} + q^+ + q^0) + f(\bar{x}) = \frac{1}{2}z^T Qz + q^0 z + f(\bar{x})$ [back]

- ▶ We know that $f(z) = z^T Qz + f(\text{bar}x)$, with $z = x - \bar{x}$. For $x \in \bar{x} + v$, with $v \in \ker(Q)$, $z = x - \bar{x} = \bar{x} + v - \bar{x} = v$. Hence $f(z) = f(\bar{x})$. On the other hand, $f(z) \geq f(\bar{x})$ for all z since $Q \succeq 0$, thus any such point is a minimum. Any point $x \in \bar{x} + v$ with $v \notin \ker(Q)$ has $f(x) = v^T Qv + f(\bar{x}) > f(\bar{x})$ since $v^T Qv > 0$ [back]
- ▶ No, this is both too trivial and didactic [back]
- ▶ $\varphi(\alpha) = a\alpha^2 + b\alpha$ quadratic non-homogeneous with $a = (g^i)^T Q g^i \geq 0$ and $b = -\|g^i\|^2 < 0$. If $a > 0$, then $\varphi(\bar{\alpha}) < \varphi(0) = f(x^i) \forall \bar{\alpha} \in (0, -b/a)$; in particular, $\bar{\alpha} = \|g^i\|^2 / (2(g^i)^T Q g^i)$ is the minimum of φ . If $a = 0$ then φ is decreasing and $\varphi(\bar{\alpha}) < \varphi(0) = f(x^i) \forall \bar{\alpha} > 0$ [back]
- ▶ The variational characterization of the eigenvalues implies that $\lambda_1 \geq d^T Qd / \|d\|^2 \geq \lambda_n$ for all $d \neq 0$; this immediately gives $1/\lambda_1 \leq \|d\|^2 / d^T Qd \leq 1/\lambda_n$ for all d , and therefore in particular $d = g^i$ (knowing that $g^i \neq 0$ otherwise the algorithm would have stopped) [back]

- ▶ The issue clearly is $g^T Qg = 0$ (very small), which means that $\varphi_{x,-g}$ is (almost) linear, and therefore f is unbounded below. One should therefore add a line
if($g^T Qg \leq \delta$) then break;
for a “very small” δ , but also add a proper way for the algorithm to signal that the returned x is not optimal, e.g., by also returning a “status code” [back]
- ▶ Having added the extra check above, the code just works: if $g^T Qg < 0$ then $(-)g$ is direction where φ has negative curvature, which still implies f is unbounded below. Note that this is not guaranteed to happen [back]
- ▶ Because $a < 0$, the step α will be negative, which basically means one is going in direction g rather than $-g$. The algorithm remains the same, except that the extra check above has to become $g^T Qg \geq -\delta$ [back]

- ▶ Assuming the gradient is computed in the “natural way” as $g = Q * x + q$ before the algorithm starts (i.e., with x the initial guess x^0), both quantities depending from matrix-vector products can be recovered by computing the vector $v = Q * g$. In fact, $a = g^T Qg = \langle g, v \rangle$. Then, with $x' = x - \alpha g$ one has $g' = Qx' + q = Q(x - \alpha g) + q = (Qx + q) - \alpha Qg = g - \alpha v$. Hence, the gradient at the next iteration can be computed in $O(n)$ out of that of the previous iteration and the vector v . As for the objective function,
$$\frac{1}{2}x^T Qx + \langle q, x \rangle = \frac{1}{2}(x^T Qx + 2\langle q, x \rangle) = \frac{1}{2}x^T(Qx + q + q) = \frac{1}{2}\langle q + g, x \rangle$$
, i.e., it can be computed in $O(n)$ once g is known [back]
- ▶ $g^i = Q(x^i - x_*) = Qx^i + q$, $\alpha^i = \|g^i\|^2 / [(g^i)^T Qg^i]$
$$g^{i+1} = Qx^{i+1} + q = Q(x^i - \alpha^i g^i) + q = (I - \alpha^i Q)g^i \implies \langle g^{i+1}, g^i \rangle = \|g^i\|^2 - \alpha^i[(g^i)^T Qg^i] = 0$$
 [back]

- ▶ All arguments boil down to the crucial $Qx^* + q = 0$. This first of all gives that $f(x^*) = \frac{1}{2}(x^*)^T Qx^* + \langle x^*, q \rangle = (x^*)^T Qx^* + \langle x^*, q \rangle - \frac{1}{2}(x^*)^T Qx^* = (x^*)^T(Qx^* + q) - \frac{1}{2}(x^*)^T Qx^* = -\frac{1}{2}(x^*)^T Qx^*$. Then, $\frac{1}{2}(x - x^*)^T Q(x - x^*) = \frac{1}{2}x^T Qx + \frac{1}{2}(x^*)^T Qx^* - x^T(Qx^*) = \frac{1}{2}x^T Qx - \langle x, q \rangle + \frac{1}{2}(x^*)^T Qx^* = f(x) - f(x^*)$ (in the penultimate step we have used $Qx^* = -q$) [back]
- ▶ Just induction: obvious for $i = 0$, if it holds for $i - 1$ then $A(x^i) \leq rA(x^{i-1}) \leq r(r^{i-1}A(x^0))$ [back]
- ▶ Q nonsingular $\implies x^i - x_* = Q^{-1}g^i \implies a^i = \frac{1}{2}(x^i - x_*)^T Q(x^i - x_*) = \frac{1}{2}(g^i)^T Q^{-1}g^i \implies a^{i+1} = \frac{1}{2}(x^{i+1} - x_*)^T Q(x^{i+1} - x_*) = \frac{1}{2}(x^i - \alpha^i g^i - x_*)^T g^{i+1} = \frac{1}{2}(x^i - x_*)^T g^{i+1}$
 [using $\langle g^{i+1}, g^i \rangle = 0$] $= \frac{1}{2}(x^i - x_*)^T Q(x^i - \alpha^i g^i - x_*)$
 $= \frac{1}{2}(x^i - x_*)^T Q(x^i - x_*) - \frac{1}{2}\alpha^i(x^i - x_*)^T Qg^i = a^i - \frac{1}{2}\alpha^i \|g^i\|^2$
 [using $Q(x^i - x_*) = g^i$] $= a^i - \frac{1}{2}\|g^i\|^4 / (g^i)^T Qg^i$

$$= a^i - \frac{\|g^i\|^4}{((g^i)^T Q g^i)((g^i)^T Q^{-1} g^i)} = a^i \left(1 - \frac{\|g^i\|^4}{((g^i)^T Q g^i)((g^i)^T Q^{-1} g^i)}\right) \quad [\text{back}]$$

- ▶ Recall $1/\lambda_n \geq \dots \geq 1/\lambda_1 > 0$ eigenvalues of Q^{-1} ; from the usual $\lambda_n \|x\|^2 \leq x^T Q x \leq \lambda_1 \|x\|^2$ (applied to Q^{-1} as well) one has $\|g\|^2 / g^T Q g \geq 1/\lambda_1$ and $\|g\|^2 / g^T Q^{-1} g \geq 1/[1/\lambda_n]$ **[back]**
- ▶ $r^k v_1 \leq \varepsilon \equiv r^k \leq \varepsilon / v^1 \equiv \log(r^k) \leq \log(\varepsilon / v^1)$ (\log monotone) $\equiv k \log(r) \leq \log(\varepsilon / v^1)$ (\log property); since $r < 1$, $\log(r) < 0$, giving $k \geq \log(\varepsilon / v^1) / \log(r) = [-\log(\varepsilon / v^1)] / [-\log(r)] = \log(v^1 / \varepsilon) / \log(1/r) = \log(v^1 / \varepsilon)[1 / \log(1/r)]$ **[back]**
- ▶ This requires a bit of elementary calculus. The derivative of $\ln(x)$ is $1/x$. The first-order Taylor approximation is $f(x + \delta) \approx f(x) + f'(x)\delta$ for $\delta \approx 0$. Applied to $\ln(\cdot)$ with $x = 1$ gives $\ln(1 + \delta) \approx \delta$, whence $1 / \ln(1/r) = 1 / \ln(1 + (1 - r)/r) = r / (1 - r)$. But $\log_a(x) = \log_b(x) / \log_b(a)$, hence $\ln(x) = \log_e(x) = \log_{10}(x) / \log_{10}(e) \approx \log(x) / 0.43 \approx 2.3 \log(x)$, i.e., $\ln(x) \in O(\log(x))$ **[back]**

- ▶ $\lambda_1 \|x^i - x_*\|^2 \geq (x_i - x_*)^T Q(x_i - x_*) = 2a^i \equiv \|x^i - x_*\| \geq \sqrt{2a^i / \lambda_1}$,
hence $d^i \leq \varepsilon \implies a^i \leq \lambda_1 \varepsilon^2 / 2$ [back]
- ▶ $a^i = \frac{1}{2}(x^i - x_*)^T Q(x^i - x_*) = \frac{1}{2}\langle g^i, x^i - x_* \rangle \leq \frac{1}{2}\|g^i\|\|x^i - x_*\|$. On the other hand, $\|g^i\|^2 = (x^i - x_*)^T Q^T Q(x^i - x_*) \geq \lambda_n^2 \|x^i - x_*\|^2$ (recall λ_n^2 eigenvalue of Q^2 , clearly the smallest), i.e., $\|g^i\| \geq \lambda_n \|x^i - x_*\|$. Hence, $\|g^i\| \leq \sqrt{2\lambda_n \varepsilon} \implies \varepsilon \geq \frac{1}{2\lambda_n} \|g^i\|^2 \geq \frac{1}{2}\|g^i\|\|x^i - x_*\| \geq a^i$ [back]
- ▶ If $f_* = -\infty$, $f_i \rightarrow -\infty$ is OK (minimising sequence) but $a^i = a^{i+1} = \infty$ and therefore their ratio is not well-defined. Since f is continuous, $\{d^i\} \rightarrow 0 \implies \{a^i\} \rightarrow 0$, but the converse need not happen in general: say, $\{x^{2i}\} \rightarrow x'_*$ and $\{x^{2i+1}\} \rightarrow x''_*$ with $x'_* \neq x''_*$ optimal solutions [back]
- ▶ Simply, $\lim_{x \rightarrow 0} x^p / x = \lim_{x \rightarrow 0} x^{p-1} = 0$: the numerator goes to 0 faster than the denominator [back]