Part 1

Examples of optimization problems

What is an optimization problem?

Mathematically speaking:

Let X be a Banach space (e.g., R^n); let

$$f: X \to R \cup \{+\infty\}$$

$$g: X \to R^{ne}$$

$$h: X \to R^{ni}$$

be functions on X, find $x \in X$ so that

$$f(x) \Rightarrow \min!$$

 $g(x) = 0$
 $h(x) \ge 0$

Questions: Under what conditions on X, f, g, h can we guarantee that (i) there is a solution; (ii) the solution is unique; (iii) the solution is stable.

What is an optimization problem?

In practice:

- *x*={*u*,*y*} is a set of design and auxiliary variables that completely describe a physical, chemical, economical model;
- f(x) is an objective function with which we measure how good a design is;
- g(x) describes relationships that have to be met exactly (for example the relationship between y and u)
- h(x) describes conditions that must not be exceeded

Then find me that *x* for which

$$f(x) \rightarrow \min!$$

 $g(x) = 0$
 $h(x) \ge 0$

Question: How do I find this *x*?

What is an optimization problem?

Optimization problems are often subdivided into classes:

Linear vs. Nonlinear

Convex vs. Nonconvex

Unconstrained vs. Constrained

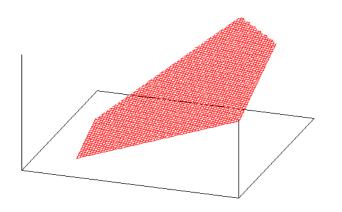
Smooth vs. Nonsmooth

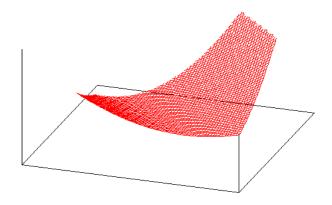
With derivatives vs. Derivativefree

Continuous vs. Discrete

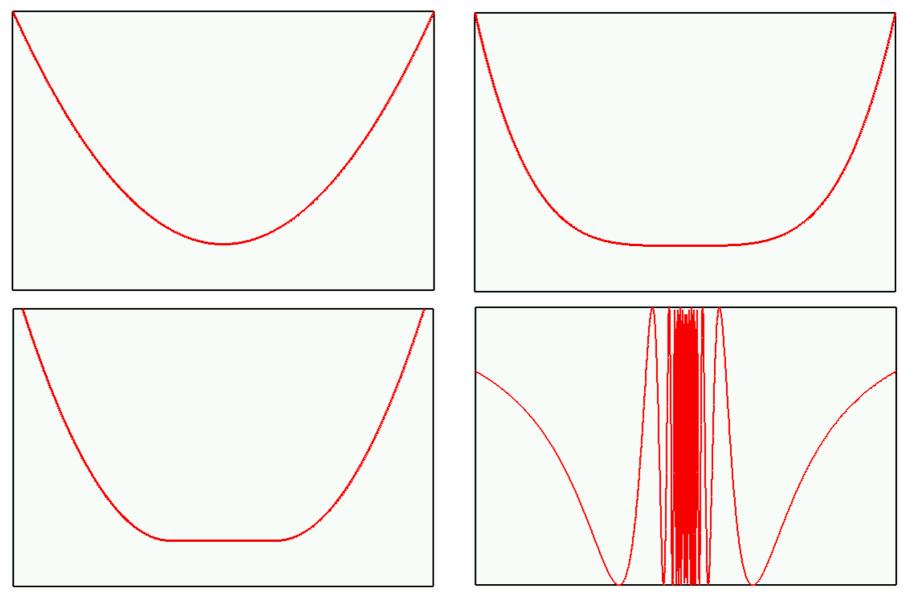
Algebraic vs. ODE/PDE

Depending on which class an actual problem falls into, there are different classes of algorithms.

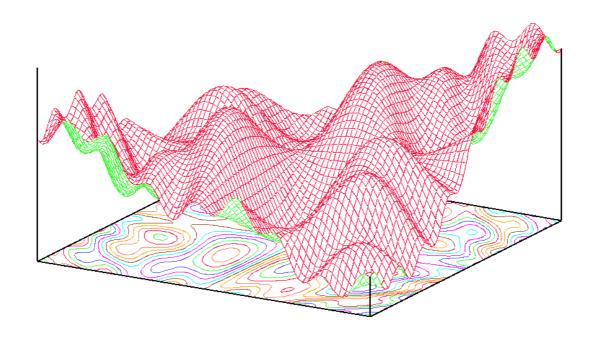




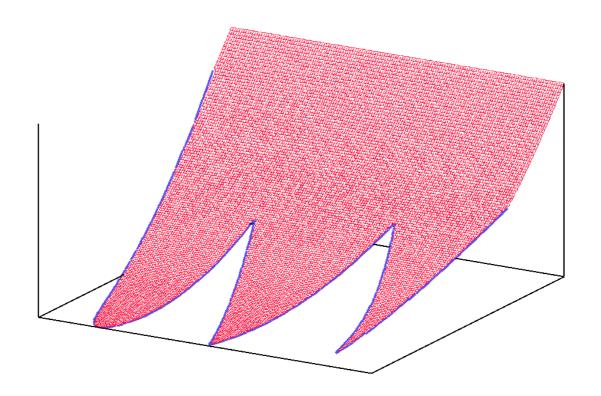
Linear and nonlinear functions f(x) on a domain bounded by linear inequalities



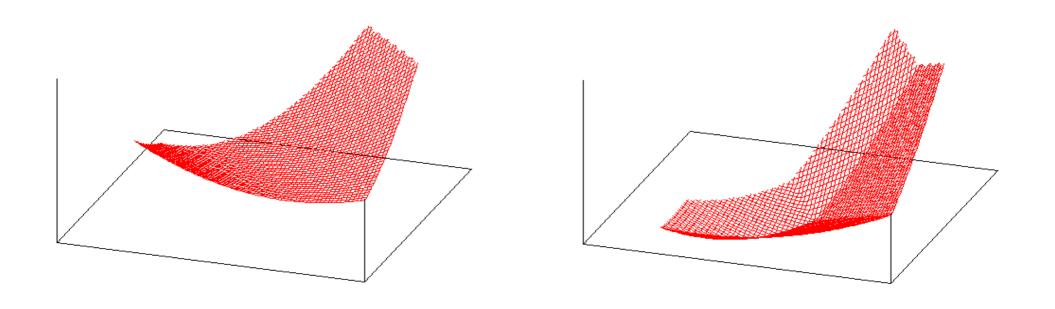
Strictly convex, convex, and nonconvex functions f(x)



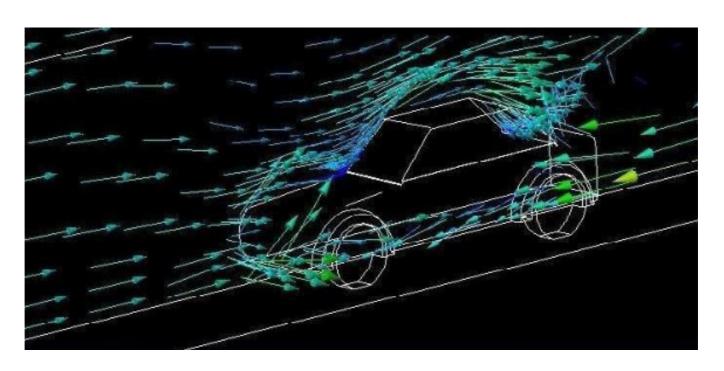
Another non-convex function with many (local) optima. We may want to find the one *global* optimum.



Optima in the presence of (nonsmooth) constraints.



Smooth and non-smooth nonlinear functions.



Mathematical description:

 $x=\{u,y\}$ u are the design parameters (e.g. the *shape* of the car) y is the flow field around the car

f(x): the drag force that results from the flow field

g(x)=y-q(u)=0

constraints that come from the fact that there is a flow field y=q(u) for each design. y may, for example, satisfy the Navier-Stokes equations

Wolfgang Bangerth

Inequality constraints:

(expected sales price – profit margin) - $cost(u) \ge 0$



volume(u) – volume(me, my wife, and her bags) ≥ 0



material stiffness * safety factor

- max(forces exerted by y on the frame) ≥ 0

Analysis:

linearity: f(x) may be linear

g(x) is certainly nonlinear (Navier-Stokes equations)

h(x) may be nonlinear

convexity: ??

constrained: yes

smooth: f(x) yes

g(x) yes

h(x) some yes, some no

derivatives: available, but probably hard to compute in practice

continuous: yes, not discrete

ODE/PDE: yes, not just algebraic

Remark:

In the formulation as shown, the objective function was of the form

$$f(x) = c_{d}(y)$$

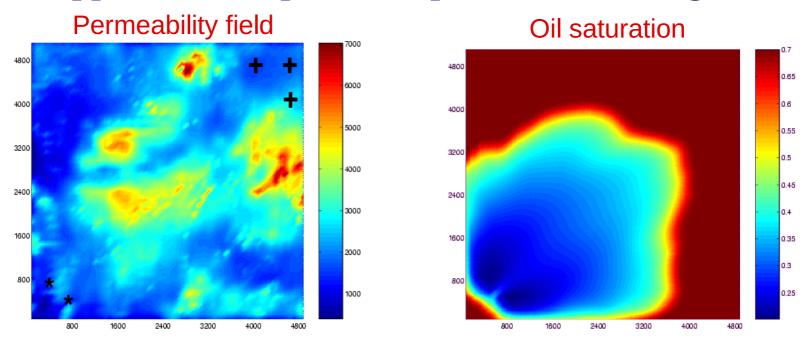
In practice, one often is willing to trade efficiency for cost, i.e. we are willing to accept a slightly higher drag coefficient if the cost is smaller. This leads to objective functions of the form

$$f(x) = c_{d}(y) + a \cos(u)$$

or

$$f(x) = c_{d}(y) + a[\cos(u)]^{2}$$

Applications: Optimal oil production strategies



Mathematical description:

 $x=\{u,y\}$ u are the pumping rates at injection/production wells y is the flow field (pressures/velocities)

f(x) the cost of production and injection minus sales price of oil integrated over lifetime of the reservoir

g(x)=y-q(u)=0

constraints that come from the fact that there is a flow field y=q(u) for each u. y may, for example, satisfy the multiphase porous media flow equations Bangerth

Applications: Optimal oil production strategies

Inequality constraints $h(x) \ge 0$:

$$U_{imax}-u_{i} \ge 0$$
 (for all wells *i*):
Pumps have a maximal pumping rate/pressure

produced_oil(T)/available_oil(0) – $c \ge 0$: Legislative requirement to produce at least a certain fraction

$$c_w$$
 - water_cut(t) ≥ 0 (for all times t):
It is inefficient to produce too much water

pressure $-d \ge 0$ (for all times and locations): Keeps the reservoir from collapsing

Applications: Optimal oil production strategies

Analysis:

linearity: f(x) is nonlinear

g(x) is certainly nonlinear

h(x) may be nonlinear

convexity: no

constrained: yes

smooth: f(x) yes

g(x) yes

h(x) yes

derivatives: available, but probably hard to compute in practice

continuous: yes, not discrete

ODE/PDE: yes, not just algebraic

Applications: Switching lights at an intersection



Mathematical description:

 $X = \{T, t_i^1, t_i^2\}$

f(x)

round-trip time *T* for the stop light system,

switch-green and switch-red times for all lights i

number of cars that can pass the intersection per

hour; to be maximized.

Note: unknown as a function, but we can measure it

Applications: Switching lights at an intersection

Inequality constraints $h(x) \ge 0$:

$$300 - T \ge 0$$
:

No more than 5 minutes of round-trip time, so that people don't have to wait for too long

$$t_i^2 - t_i^1 - 5 \ge 0$$
:

At least 5 seconds of green at each light *i*

$$t_{i+1}^1 - t_i^2 - 5 \ge 0$$
:

At least 5 seconds of all-red between different greens

Applications: Switching lights at an intersection

Analysis:

linearity: f(x) ??

h(x) is linear

convexity: ??

constrained: yes

smooth: f(x)??

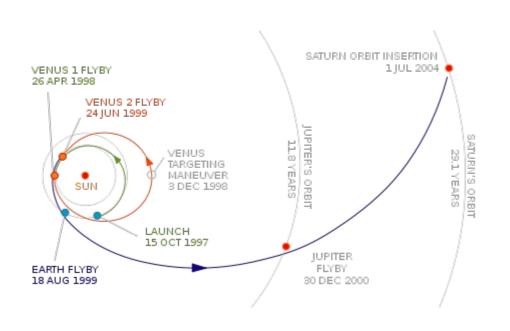
h(x) yes

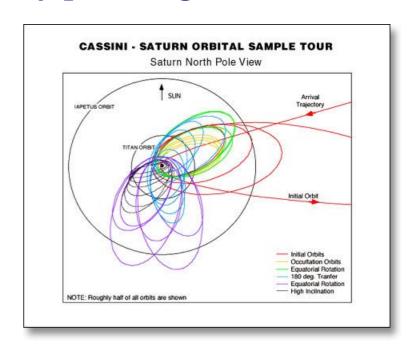
derivatives: not available

continuous: yes, not discrete

ODE/PDE: no

Applications: Trajectory planning





Mathematical description:

 $x=\{y(t),u(t)\}$ position of spacecraft and thrust vector at time t $f(x)=\int_0^T |u(t)|dt$ minimize fuel consumption

$$m \ddot{y}(t) - u(t) = 0$$
 Newton's law $|y(t)| - d_0 \ge 0$ Do not get too close to the sun $u_{\max} - |u(t)| \ge 0$ Only limited thrust available

Applications: Trajectory planning

Analysis:

linearity: f(x) is nonlinear

g(x) is linear

h(x) is nonlinear

convexity: no

constrained: yes

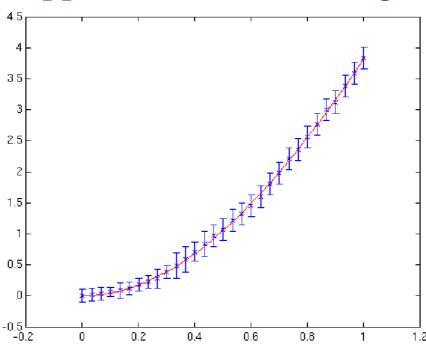
smooth: yes, here

derivatives: computable

continuous: yes, not discrete

ODE/PDE: yes

Note: Trajectory planning problems are often called *optimal* control.



Mathematical description:

$$x=\{a,b\}$$
 parameters for the model $y(t)=\frac{1}{a}\log\cosh(\sqrt{ab}\,t)$
 $f(x)=1/N \sum_{i} |y_{i}-y(t_{i})|^{2}$

mean square difference between predicted value and actual measurement

Analysis:

linearity: f(x) is nonlinear

convexity: ?? (probably yes)

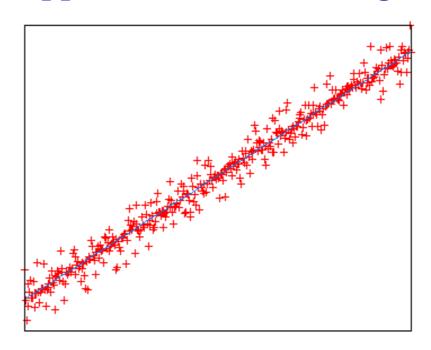
constrained: no

smooth: yes

derivatives: available, and easy to compute in practice

continuous: yes, not discrete

ODE/PDE: no, algebraic



Mathematical description:

$$x=\{a,b\}$$

 $x=\{a,b\}$ parameters for the model

$$f(x)=1/N \sum_{i} |y_{i}-y(t_{i})|^{2}$$

mean square difference between predicted value and actual measurement

→ *least squares* problem

y(t)=at+b

Analysis:

linearity: f(x) is quadratic

Convexity: yes

constrained: no

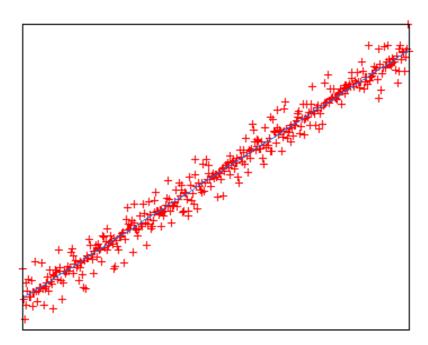
smooth: yes

derivatives: available, and easy to compute in practice

continuous: yes, not discrete

ODE/PDE: no, algebraic

Note: Quadratic optimization problems (even with linear constraints) are easy to solve!



Mathematical description:

 $x=\{a,b\}$

parameters for the model y(t)=at+b

$$f(x)=1/N \sum_{i} |y_{i}-y(t_{i})|$$

mean *absolute* difference between predicted value and actual measurement

→ *least absolute error* problem

Analysis:

linearity: f(x) is nonlinear

Convexity: yes

constrained: no

smooth: no!

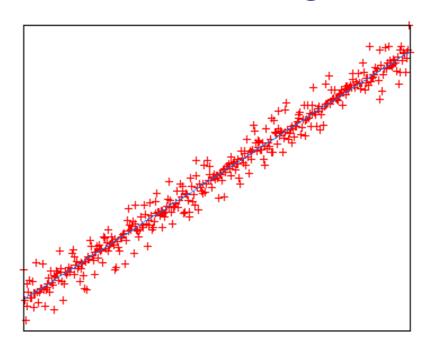
derivatives: not differentiable

continuous: yes, not discrete

ODE/PDE: no, algebraic

Note: Non-smooth problems are really hard to solve!

Applications: Data fitting 3, revisited



Mathematical description:

 $x=\{a,b,s\}$ parameters for the model y(t)=at+b"slack" variables s_i

$$f(x)=1/N \sum_{i} s_{i} \rightarrow \min!$$

$$|S_i - |y_i - y(t_i)| \ge 0$$

$$y(t) = at + b$$

Applications: Data fitting 3, revisited

Analysis:

linearity: f(x) is linear, h(x) is not linear

Convexity: yes

constrained: yes

smooth: no!

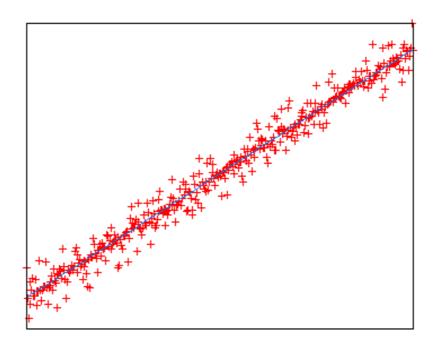
derivatives: not differentiable

continuous: yes, not discrete

ODE/PDE: no, algebraic

Note: Non-smooth problems are really hard to solve!

Applications: Data fitting 3, re-revisited



Mathematical description:

$$x=\{a,b,s\}$$

parameters for the model y(t)=at+b

"slack" variables s_i

$$f(x)=1/N \sum_{i} s_{i} \rightarrow \min!$$

$$s_i - |y_i - y(t)| \ge 0$$

$$S_i - (y_i - y(t_i)) \ge 0$$

$$S_i + (y_i - y(t_i)) \ge 0$$

Applications: Data fitting 3, re-revisited

Analysis:

linearity: f(x) is linear, h(x) is now also linear

Convexity: yes

constrained: yes

smooth: yes

derivatives: yes

continuous: yes, not discrete

ODE/PDE: no, algebraic

Note: Linear problems with linear constraints are simple to solve!

Applications: Traveling salesman



Task: Find the shortest tour through N cities with mutual distances d_{ij} .

(Here: the 15 biggest cities of Germany; there are 43,589,145,600 possible tours through all these cities.)

Mathematical description:

 $X = \{C_i\}$

the index of the *i*th city on our trip, i=1...N

$$f(x) = \sum_{i} d_{c_i c_{i+1}}$$

 $c_i \neq c_j$ for $i \neq j$ no city is visited twice (alternatively: $c_i c_j \geq 1$)

Applications: Traveling salesman

Analysis:

linearity: f(x) is linear, h(x) is nonlinear

Convexity: meaningless

constrained: yes

smooth: meaningless

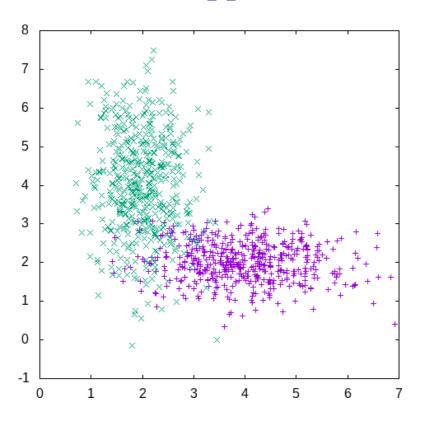
derivatives: meaningless

continuous: discrete: $x \in X \subset \{1,2,...,N\}^N$

ODE/PDE: no, algebraic

Note: Integer problems (combinatorial problems) are often exceedingly complicated to solve!

Applications: Classification problems



Task: Find a line that as best as possible separates the two known data sets.

Goal: When a new point comes in, be able to *classify* it with high probability as either green or purple.

Challenge: This often happens in very high dimensions.

Mathematical description:

$$x=\{a,b\}$$

Coefficients of the line y=ax+b

f(x)

Number of misclassified green/purple points

Applications: Classification problems

Analysis:

linearity: f(x) is nonlinear – in fact, it is a step function!

Convexity: no

constrained: no

smooth: no

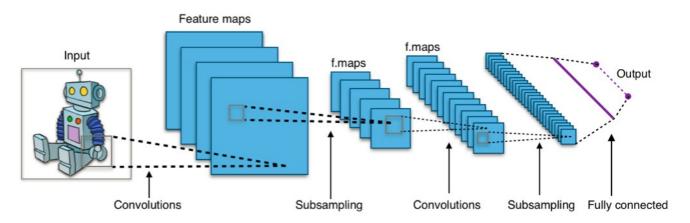
derivatives: no (step function)

continuous: yes, not discrete

ODE/PDE: no, algebraic

Note: Non-smooth problems are difficult to solve. We may do well reformulating the problem to something smooth.

Applications: Neural networks



Method: Each layer of the NN can be thought of as a parameterized function with inputs from the previous layer.

Task: Find parameters so that we get desired outputs for known inputs.

Mathematical description:

 x_{ij}^n Parameters of node i,j of layer n

f(x) Average difference between desired and obtained classification

Applications: Neural networks

Analysis:

linearity: f(x) is nonlinear

Convexity: ?

constrained: maybe (e.g. if weights have to be positive)

smooth: yes

derivatives: depends on formulation

continuous: yes, not discrete

ODE/PDE: no, algebraic

Part 2

Minima, minimizers, sufficient and necessary conditions