Artelys | OPTIMIZATION SOLUTIONS

KNITRO®

Solving black box models with a derivative based nonlinear optimization solver

JFRO 2024

Paris

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www.artelys.com

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Artelys

Artelys is an independent company, created in 2000, specialized in optimization, decision-support, modeling.

2000
CREATION
Arnaud Renaud

15% annual
sustained growth

120 EXPERTS
MSc and PhD

25% of our activity
is dedicated to R&D

SOFTWARE EDITION
Custom software,
off-the-shelf software,
Numerical solvers

SERVICES & CONSULTING
Optimisation,
Data Science
and business expertise

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Artelys Knitro overview

Some historical background

- Created in 2001 by Ziena Optimization
  - ↳ Spin-off of Northwestern University
- Artelys is the worldwide distributor of Knitro since 2009
- Artelys acquired Ziena Optimization in 2015

Key features

- Efficient and robust solution on **large scale** problems (~10^5 variables)
- Four active-set and interior-point algorithms for continuous optimization
- MINLP algorithms and complementarity constraints for discrete optimization
- Many extra features based on **customer feedbacks** or project requirements
- Parallel multi-start method for global optimization.
- Easy to use and well documented: Online documentation

Artelys Knitro problem classes solved

$$
\begin{aligned}
\min_{x\in\mathbb{R}^n, y\in\mathbb{Z}^m} \quad & f(x,y) & \\
\text{s.t.} \quad & g_i(x,y) \geq 0 & i \in I \\
& h_j(x,y) = 0 & j \in J \\
& 0 \leq x_k \perp x_l \geq 0 & (k,l) \in C \subset [\![1,n]\!]^2 \\
& l_x \leq x \leq u_x & \\
& l_y \leq y \leq u_y &
\end{aligned}
$$

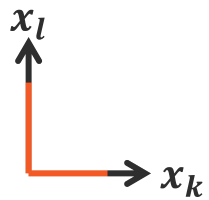
Variables (x and y)

- Continuous or discrete
- Bounded or unbounded

Objective (f) and constraints (g and h)

- Algebraic equations available or external callback to evaluate functions (**black box**)
- Smoothness: preferred but not required
- Convexity: preferred but not required, local optimization or global optimization with multistart

Complementarity constraints



- $0 \leq x_k \perp x_l \geq 0$ is equivalent to: $x_k \geq 0$ and $x_l \geq 0$ and $\{x_k = 0 \text{ or } x_l = 0\}$
- Applications: strategic bidding, economic models, equilibrium constraints, disjunctions

Artelys Knitro overview

Interfaces

- Modeling languages
- Programming languages

Supported platforms

Windows 64-bit

Linux 64-bit

macOS 64-bit

ARM architecture

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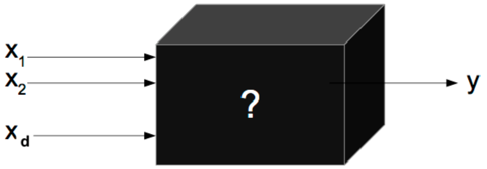
Black box – General overview

Artelys Knitro is widely used to solve black box applications

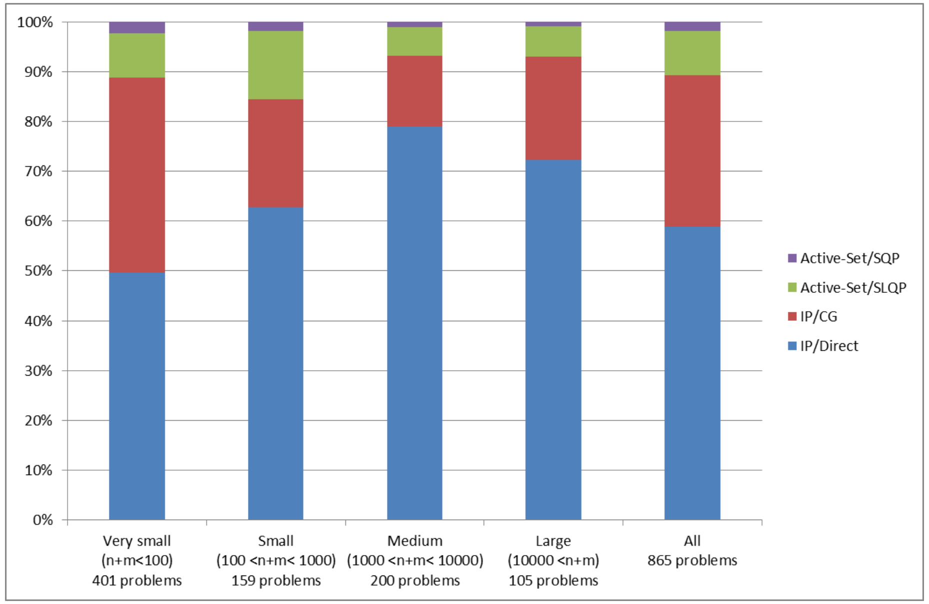
- Grey / Black box applications arise when the algebraic equations of the optimization model is not known or only partially



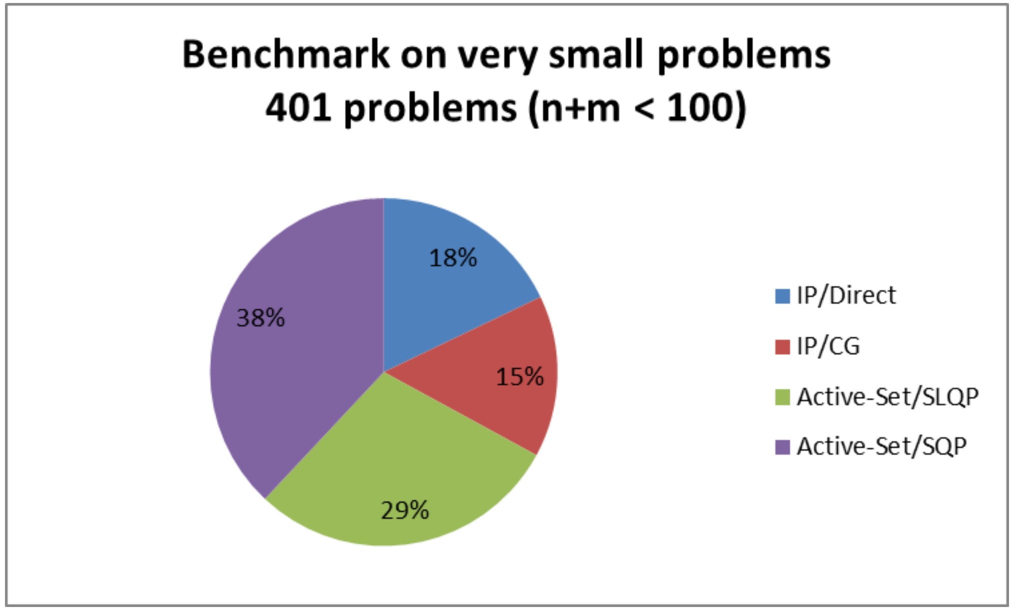
- Most of the time the optimization relies on an external simulator to compute the model state
  - Blending models – oil&gas, mining industry …
  - Finite elements computations – computer aided design (CAD), electric transformers design, structure design …
  - Hydraulic models
  - Multi-Disciplinary Analysis and Optimization (MDAO)
    - Connection possible with OpenMDAO developed by Nasa
    - Major applications in spatial, aeronautics, autonomous vehicles
    - Good results obtained for industrial customers in the defense sector

Artelys Knitro algorithms comparison

Comparison on Artelys Knitro four different algorithms



Exact first and second order derivatives



Derivative free optimization (Black box)

Advantage of active set methods for black box models

- Converge in fewer iterations (minimize the number of function evaluations)
- Good warm start

Cost of derivative approximation (1)

Approximation of first derivatives by finite differences (biggest cost)

- Good approximation necessary for the convergence of the algorithms

- Forward or central finite differences – tradeoff that is not always obvious !
  - Central brings accuracy than can cut down iterations significantly !

- Automatic selection of the finite differences step to avoid falling in the simulator noise
  - 1e-15 by default for algebraic equations, can be changed by user
  - E.g. for transformer design, changing the size of the transformer by 1e-15 is not significant

- Can also exploit the sparsity pattern of the Jacobian if available.
  - Even if it is black box, not all constraints depend on all variables -> physical knowledge of the simulator

- Ability to perform parallel function evaluations to compute finite differences

Cost of derivative approximation (2)

- Approximation of the Hessian (second-order derivative)
  - These methods do not require additional function evaluations.
  - Improve convergence “for free” (in terms of function evaluation)

- Possibility to pass the known structure separately (linear, quadratic, conic..)
  - Knitro can compute the exact derivatives of several expressions
  - Part of the model can be black box and approximated, the rest can be passed as algebraic equations
  - For example:
    - Pass linear structure directly to Knitro
    - Create one callback with nonlinear expressions for which you can pass derivatives (at least Jacobian)
    - Create one ‘black box’ callback where no derivatives can be provided

Other nice features

- Noise estimation to allow faster convergence by analyzing the simulator precision
  - Automatic update of termination criteria when iteration steps reaches estimated simulator precision

- Ability to multistart for non-convex models to use different initial points
  - Initial points can be provided by the user or automatically generated
  - Specific convergence criteria to stop when probability to find a new local solution is low

- Specific MISQP algorithm for problem with non relaxable integers
  - Do not rely on a B&B approach
  - Particularly interesting for physical simulators with strong integrity constraint on parameters
  - Mimic SQP continuous algorithm relying on a grid search for integer variables

Achievements

- Consistently getting good results on Black-box competition (BBCOMP) from 2016 to 2019
  - Won several single objective and multi-objective instances over the years
  - Especially on expensive tracks with limited function evaluation budget
  - Simple plugin of Knitro relying on the different features
    - Multi start was activated to start from different initial points
    - Management of termination criteria to avoid spending effort on low quality solves
    - For multi-objective, we recreate the “pareto front” by successively optimizing the different objectives

- Since we participated in BBCOMP
  - Automatic step computation of finite differences
  - Noise estimation for convergence criteria
  - Ability to pass some of the problem structure when available
  - Enhanced multistart initial point generation and termination criteria

- Always open to new challenges if you have any !

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Conclusion

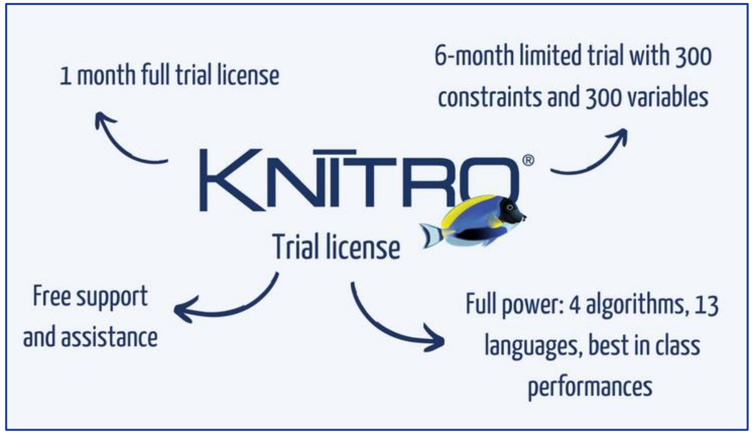
Summary

- Artelys Knitro provides several competitive specialization for black box models
- First order derivative approximation is the predominant cost (because of function evaluations)
- Pass as much information as you can, it's not necessarily equations !
- Knitro will approximate all the required information you can't provide
- Particularly efficient for applications with strict computation budget !

Future developments will continue focusing on improving Black box features

- Automatic detection of sparsity pattern for Jacobian approximation
- Approximate several independent Jacobian values simultaneously

Come and try it !

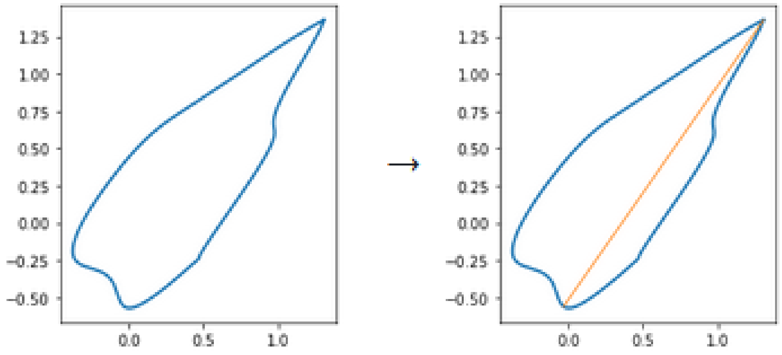


Free trial

- Directly accessible from our website

Free teaching program

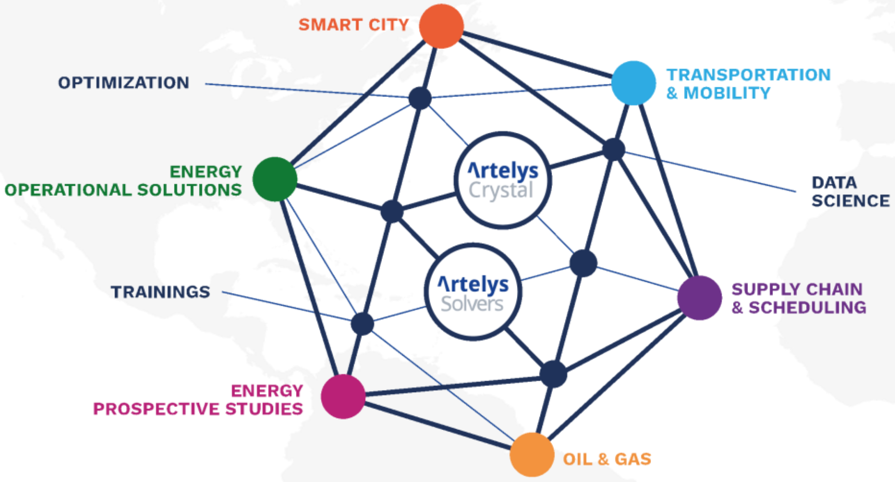
- Free academic licenses for the professor and the students during the time of the course
- Contact us at info-knitro@artelys.com



Checkout Artelys Knitro tutorials on Github

- Include models both with Knitro API or modeling languages !
- https://github.com/Artelys/knitro-modeling-examples

Contact



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