A modeling-language based approach to automatically recommend optimization methods

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#### Motivating example: LASSO regression

Consider  $X \in \mathbb{R}^{n \times d}$ ,  $y \in \mathbb{R}^{n}$ ,  $\lambda_{1}$ ,  $\lambda_{2}$ ,  $\lambda_{3} \in \mathbb{R}_{+}^{*}$ . LASSO regression solves:

$$\hat{\beta} \in \arg\min_{\beta \in \mathbb{R}^d} \left\{ \frac{1}{2} \|y - X\beta\|^2 + \lambda_1 \|\beta\|_1 \right\}, \qquad (\text{nonsmooth convex})$$

or equivalently,

$$\hat{\beta} \in \arg\min_{\beta \in \mathbb{R}^d} \left\{ \frac{1}{2} \|y - X\beta\|^2 \text{ subject to } \|\beta\|_1 \le \lambda_2 \right\}$$
(QP)

or equivalently,

$$\hat{\beta} \in \arg\min_{\beta \in \mathbb{R}^d} \left\{ \|\beta\|_1 \text{ subject to } \|y - X\beta\|^2 \le \lambda_3 \right\}$$
(SOCP)

For each formulation, you can use many different methods:

Some applicable methods
coordinate descent, subgradient method, proximal gradient
splitting methods, active-set methods
augmented lagrangian, splitting methods

Four steps approach

- So. Gather methods with associated complexity results
- S1. *Match* a given formulation with all applicable methods
- S2. *Reformulate* a given problem to find equivalent formulations
- S3. Compare complexity results of (formulation, method) combinations

### In this talk

We present the Optimization Methods Ranking Assistant (OMRA)

- A repository of convergence results existing in the literature
- A modeling language to describe optimization problems
- Detection of methods applicable to user-provided problems
- Comparison of applicable methods by worst-case performance
- ▶ all of this framed in a Python toolbox.

#### Pipeline



#### Outline

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### Setting : What optimization problems usually look like

#### Consider any optimization problem in the black-box form:

$$\min_{x} f(x) \tag{1}$$

where f is decomposed into simpler components  $f_i$ , for example:

$$f(x) = f_1(x) + f_2 \circ f_3(x) + \sum_{j=1}^n f_4^j(x) - \max_{j=1,\dots,n} f_5^j(x)$$
(2)

with

- possible assumptions on the f<sub>i</sub>'s (convexity, Lipschitz continuity, etc.)
- ▶  $f_i$  can also correspond to "atom functions":  $\ell_1$ -norm ...
- access to certain oracles for each f<sub>i</sub> (subgradient, proximal operator, etc.)

### Example of what you can find in the literature

Theorem: Worst-case convergence rate of Fast Proximal Gradient Method

Take  $f : \mathbb{R}^n \to \mathbb{R}$  *L*-smooth and convex and  $h : \mathbb{R}^m \to \mathbb{R}$  closed, proper, convex. Suppose  $||x_0 - x_*|| \le R$ . Then, the Fast Proximal Gradient Method with stepsize  $\frac{1}{L}$  applied to minimizing F(x) = f(x) + h(x) satisfies for all  $n \ge 1$ :

$$F(x_n) - F(x_*) \le \frac{2L}{n^2 + 5n + 2} ||x_0 - x_*||^2$$
(3)

## Complexity results follow the same skeleton

Theorem: Worst-case convergence rate of Algorithm 1

Suppose assumptions  $\{(A1), (A2), (A3)\} = \mathcal{A}$  hold. Consider some initial conditions  $\mathcal{I}$ . Then, Algorithm 1 with parameters  $\mathcal{P}$  applied to Problem (1) satisfies for all  $k \ge 1$ 

$$F(x_k) - F(x^*) \le \varphi(k, \mathcal{A}, \mathcal{I}, \mathcal{P})$$
(4)

Existing results (always) have

- Some template optimization problem (in red)
- The considered optimization method (in purple)
- A rate of convergence (in green)

### Elements to encode known complexity results

#### **Template problem**

This is just an optimization problem (use a modeling language)
 Optimization method

- Enough to encode the parameters.
- > Dependence of method parameters to template parameters

#### **Convergence rate**



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### How to write an optimization problem in OMRA

Problem

$$\min_{x\in\mathbb{R}^n} f(x) + g(A(x))$$
 (5)

where

- ►  $f : \mathbb{R}^n \to \mathbb{R}$  is convex, *L*<sub>f</sub>-smooth. Access to  $\nabla f$ .
- ▶  $g : \mathbb{R}^m \to \mathbb{R}$  is convex. Access to *prox*<sub>g</sub>.
- ►  $A : \mathbb{R}^n \to \mathbb{R}^m$  is a linear mapping with  $||A|| \le M$ . Access to  $x \to Ax$ .

pb = Problem() x = pb.declare\_variable("x", Rn)  $f = pb.declare_function("f", Rn, R)$ g = pb.declare\_function("g", Rm, R)  $A = pb.declare_function("A", Rn, Rm)$ pb.set\_objective(f(x) + g(A(x))) f.add\_property(Convex()) f.add\_property(Smooth(0, 10.)) g.add\_property(Convex()) A.add\_propertv(Linear(10.)) pb.declare\_oracle(Derivative(f)) pb.declare\_oracle(Proximal(g)) pb.declare\_oracle(Evaluation(A))

#### Optimization problem as a Directed Acyclic Graph



#### Optimization problem as a Directed Acyclic Graph



#### Optimization problem as a Directed Acyclic Graph







f(x) + g(x)f(x) + g(x)f(x) + g(x)+ + f(x)g(x)f(x)g(x)@ @ @ @  $f f' \in \partial f$ Х  $g \nabla g$  $f f' \in \partial f$ X g X  $\nabla g$ Х Strongly convex *L*-smooth Convex *L*-smooth Optimization Template T Optimization Problem P











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### Scenario 2 : reformulations

We need to match user-provided problems to templates.

- ✓ Ideal scenario is immediate match of user-provided problem to template.
- ► Solution otherwise: use *mathematical results and reformulation tricks* !

#### Mathematical results:

- Sum of smooth (resp. convex) functions is smooth (resp. convex),
- ► Proximal operator of  $f + \gamma ||x||^2$  is computable given  $prox_f$  ...

#### Reformulation tricks:

- ► Commutativity of operators,
- losing structure and regrouping terms,
- transfer of curvature (parametrized reformulation),
- computing oracles as a subproblem (parametrized reformulation) ...

#### Reformulation example



#### Commutativity of the sum operator



#### Losing structure



### Transfer of curvature



#### Outline

So far: from a user-provided problem, we get a list of (Template, Method, Rate)

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#### **Our ranking criterion:**

The convergence rate associated to each (template, method) combination (× *the computational cost per iteration*)

### How to deal with sophisticated rate functions

Example: Convergence rate of fixed-step ( $\gamma$ ) GD for f convex and L-smooth

$$f(x_N) - f_* \leq \frac{L}{2} \frac{\|x_0 - x^*\|^2}{1 + \gamma L \min\left\{2N, \frac{-1 + (1 - \gamma L)^{-2N}}{\gamma L}\right\}}$$

- 1. Compute rates numerically whenever possible
- 2. Drop asymptotically worse methods if high iteration budget
- 3. Compare leading coefficients whenever possible
- 4. Sampling method

### **Conclusions**

Contribution: a principled approach to compare optimization methods and its Python implementation, OMRA

 Large repository of known results in the form (Template, Method, Convergence Rate)





► Make this encyclopedia available through a website (very soon)

#### Make the toolbox richer

- Aggregate more results in the database
- Add reformulation techniques ( $\eta$ -trick, duality (for the LASSO example))

#### **User features**

Code generation for recommended methods

# Thank you again for your attention!

# **Questions**?

#### Do not hesitate to contact me:

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## Preliminary results: Equivalent templates

Problem: Additive composite template

$$\min_{x \in \mathbb{R}^n} f(x) + g(x) \tag{6}$$

where

- ►  $f : \mathbb{R}^n \to \mathbb{R}$  is  $\mu_f$ -convex,  $L_f$ -smooth. Access to  $\nabla f$ .
- ▶  $g : \mathbb{R}^n \to \mathbb{R}$  is  $\mu_g$ -convex,  $L_g$ -smooth. Access to *prox*<sub>g</sub>.

# Problem: Difference of convex template

$$\min_{x\in\mathbb{R}^n}\varphi_1(x)-\varphi_2(x) \qquad (7)$$

#### where

•  $\varphi_1 : \mathbb{R}^n \to \mathbb{R}$  is convex,  $L_{\varphi_1}$ -smooth. Access to  $\nabla \varphi_1$ .

• 
$$\varphi_2 : \mathbb{R}^n \to \mathbb{R}$$
 is convex.  
Access to  $\nabla \varphi_2$ .

Through the sequence of (implemented) transformations

$$f(x) + g(x) = g(x) + f(x) (Commutativity of the sum operator)$$
(8)  

$$= (g(x) + \gamma ||x||^{2}) + (f(x) - \gamma ||x||^{2}) (Transfer of curvature)$$
(9)  

$$= (g(x) + \gamma ||x||^{2}) - (\gamma ||x||^{2} - f(x)) (plus = minus minus)$$
(10)  

$$= \varphi_{1} - \varphi_{2}.$$
(11)

- Properties: Depending on the parameter  $\gamma$ , we can make  $\varphi_1$ ,  $\varphi_2$  convex.
- Having *prox*<sub>g</sub> and  $\nabla f$ , we can compute  $\nabla \varphi_1$ ,  $\nabla \varphi_2$ .

# Full matching algorithm

```
class Problem:
  Γ...]
  def compute_reformulations(self):
    visited = set()
    queue = [self.objective]
    while len(queue):
        current_tree = queue.pop(0)
        for g in TRANSFORMATIONS:
            for new_tree in current_tree.transform(g):
                if new tree not in visited:
                    visited.add(new_tree)
                    queue.append(new_tree)
    return set(list(visited))
```