Google Summer of Code 2023 : NumFOCUS Final Report on Adding structured Lagrangian support to CVXPY

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Contents

1	Intr	roduction:	2
	Coc	ling Period:	3
	2.1	Pre-midterm evaluation:	3
	2.2	Post-midterm evaluation:	4
		2.2.1 #2204, check_dual_domains, and the introduction of	
		the dual_cone/residual methods:	4
		2.2.2 WiP on fork, _is_differentiable_at — verifying points	
		of non-differentiability:	4
	2.3	Future work:	5

1 Introduction:

This document details the contributions I made to CVXPY's codebase over the duration of my GSoC, '23 project titled: **Adding Structured Lagrangian support to CVXPY**. My work during the GSoC period was to build infrastructure for verifying the KKT conditions, in-so-far as that is concerned, we were able to implement it for all differentiable Atom classes that CVXPY supports (for the case of *stationarity checks*).

I provide the KKT conditions (and their corresponding CVXPY method) below. Again, consider a general optimization problem **P**, and it's dual **G**:

$$\begin{array}{ll}
\mathbf{P} \\
\max_{x \in \mathcal{D}} & f_0(x) \\
\text{subject to} & f_i(x) \leq 0, \quad i = 1 \dots, m \\
& h_i(x) = 0, \quad i = 1, \dots, p
\end{array}$$

$$\mathbf{G}$$

$$\max_{\lambda,\nu} \min_{x} \quad g(\lambda,\nu)$$
subject to $\lambda > 0$

Where,
$$g(\lambda, \nu) = (f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) + \sum_{i=1}^{p} \nu_i h_i(x))$$

1. Stationarity of the Lagrangian,

cvxpy/tests/solver_test_helpers.py:SolverTestHelper::
check_stationary_lagrangian

$$\mathbf{0} \in \partial \left(f_0(x) + \sum_{i=1}^m \lambda_i f_i(x) + \sum_{i=1}^p \nu_i h_i(x) \right)$$
 (1)

Here $\partial(.)$ represents the subdifferential of a function.

2. Dual feasibility,

cvxpy/tests/solver_test_helpers.py:SolverTestHelper::
check_dual_domains:

$$\lambda_i \ge 0, i = 1, 2, \dots, m \tag{2}$$

3. Complimentary Slackness,

cvxpy/tests/solver_test_helpers.py:SolverTestHelper::
check_complimentarity (existed pre-GSoC contributions):

$$\lambda_i.f_i(x) = 0, i = 1, 2, \dots, m$$
 (3)

4. Primal feasibility,

cvxpy/tests/solver_test_helpers.py:SolverTestHelper::
check_primal_feasibility (existed pre-GSoC contributions):

$$f_i(x) \le 0, i = 1, 2, \dots, m$$

 $h_i(x) = 0, i = 1, 2, \dots, p$

The implementation of all of the above constituent conditions, with the exception of check_stationary_lagrangian and check_dual_domains (for certain Constraint classes) is *complete* and general enough to encompass the majority of CVXPY's current functionality.

A lot of time was spent thinking about the particular design and implementation of the above methods since it involved major changes to the public API of CVXPY. Most of the newly implemented methods and changes will possibly be made public after the above KKT verification methods are made sufficiently general to cover all of CVXPY's current functionality.

The plan is to move the above verification methods out of SolverTestHelpers (perhaps temporarily to cvxpy/problems/kkt.py), and eventually write an instance method on the cp.Problem class that checks all of the KKT conditions and provides meaningful output in case any of the checks fail.

2 Coding Period:

2.1 Pre-midterm evaluation:

The major contribution pre-midterm was the implementation of the check--_stationary_lagrangian method.

Much of this has been documented in a blog post that can be found on my webpage, here.

But to summarize, we were able to quickly get up and running with a basic implementation that worked for the constraints in CVXPY that support

recovery of the values of the dual variables (this is done via cp.Constraint--.dual_variables to access the dual variables themselves or via cp.Constraint-.dual_value to access the values that they store. These fields are populated after a cp.Problem is successfully solved).

The tricky part with this implementation was the fact that CVXPY supports passing in implicit constraints via flags when declaring variables. Since there was no way to symbolically access these constraints, we had to be a bit clever and re-contextualize stationarity in a more general way to account for these implicit constraints. Namely the idea being that of characterizing the dual cone K^* of the convex cone K that the variable is implicitly constrained to lie in. Specifically, instead of the gradient w.r.t these variables being $\mathbf{0}$, the gradient should instead lie within K^* — hence, we had to check set membership for the computed gradients for variables with such flags.

I also made a <u>minor bug-fix</u> which I happened upon when I was working on the implementation of dual cones for the existing Constraint classes.

NOTE: The test cases for much of this functionality resides within cvxpy/tests/test_kkt.py

2.2 Post-midterm evaluation:

There were two major threads that I worked on post-midterm:

2.2.1 $\frac{\#2204}{\text{methods}}$, check_dual_domains, and the introduction of the dual_cone/residual methods:

This PR introduces several sweeping API altercations. For one, it introduces an entirely *new* Cone class which subclasses Constraint. This is a new class which all convex conic constraints now inherit from.

The reason for this change was the introduction of two new methods (which do not make any semantic sense for algebraic constraints, such as Inequality), namely, _dual_cone (private method) and dual_residual. The former returns the corresponding dual cone of the Cone instance, while the latter is just a convenient method for computing the violation on the dual variable values that CVXPY returns w.r.t K^* returned in _dual_cone — we use dual_residual within check_dual_domains.

2.2.2 <u>WiP on fork</u>, _is_differentiable_at — verifying points of non-differentiability:

This PR again adds a new method, this time, to the Atom class. The intention behind this work was the introduction of the notion of strict_differentiability

for grad computations in CVXPY.

Namely, CVXPY returns a subgradient for every atom (for which grad has been implemented), but for points of non-differentiability, the subdifferential at that point is a non-singleton set, and hence, in such cases a distinction needed to be made to the end of stationarity checks.

This PR adds several new pieces of code, for one, we implement the _is_differentiable_at method on a variety of atoms, which point out whether an atom is differentiable or not at that point (i.e., whether or not the subdifferential at that point is a singleton set). To keep the existing grad computation as parallel to the current semantics as possible, we introduce a new context manager within cvxpy/utilities/scopes.py::strict_differentiability_scope. Here is an example use case:

```
import cvxpy as cp
import numpy as np
from cvxpy.utilities.scopes import strict_differentiability_scope

X = cp.Variable(shape=(3,3))
X.value = np.zeros((3,3))
expr = cp.norm1(X)

expr.grad # does not throw an error
with strict_differentiability_scope():
    expr.grad # throws NotDifferentiableError
```

The reason the _is_differentiable_at method was wrapped around the _grad methods on every atom (and not directly on the grad method that is defined on the Atom class which implements the chain rule), is to ensure that we can naturally leverage the recursive *canonicalization* process of CVXPY parsing the expression tree (since _grad is where the computation for grad bottoms out). Similarly, in the case of AxisAtom's, we wrap the _is_differentiable_at method around the _column_grad method.

This is still a WiP, with some the _is_differentiable_at method for some atom classes requiring some changes.

2.3 Future work:

After the official period for GSoC 2023 ends, I will be extending our work as part of my thesis requirement with Dr. Riley Murray. So far, we plan on working on the following major features:

- 1. Introduce a new ConvexSet class to the end of implementing subdifferential support in CVXPY from the ground up
- 2. Implement dual variable recovery, and the _dual_cone and dual_residual methods for PowConeND
- 3. Derive the dual cone for the semidefinite approximation of the class of exotic convex cones (namely, the Relative Entropy Cone and the Operator Relative Entropy Cone) which we worked on implementing within CVXPY as part of my GSoC 2022 project.