Flexible Differentiable Optimization via Model Transformations

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Abstract

We introduce DiffOpt.jl, a Julia library to differentiate through the solution of convex optimization problems with respect to arbitrary parameters present in the objective and/or constraints. The library builds upon MathOptInterface, thus leveraging the rich ecosystem of solvers and composing well with modelling languages like JuMP. DiffOpt offers both forward and reverse differentiation modes, enabling multiple use cases from hyperparameter optimization to backpropagation and sensitivity analysis, bridging constrained optimization with end-to-end differentiable programming.

1. Introduction

Differentiable Optimization (∂O) has become a center of interest in the last years, both as a stand-alone methodology providing additional information on the sensitivity of general convex optimization problems and as a principled way to integrate complex convex optimization components in Machine Learning, following a broader trend of differentiable programming which extends the set of computer programs for which derivatives can be computed [Innes et al., 2019]. We present DiffOpt, a library implementing key methods for ∂O in Julia [Bezanson et al., 2017] based on the MathOptInterface (MOI) abstract data structure [Legat et al., 2021]. Consequently, the extensions to the usual mathematical optimization machinery are also available in JuMP [Dunning et al., 2017] with MOI as its backend.

The rest of this paper is structured as follows. Section 2 covers the background and related research on ∂O . Section 3 presents the structure of the DiffOpt package and important features. Section 4 highlights some applications illustrating the use of the package.

2. Differentiating Convex Optimization Problems

 $\partial \mathcal{O}$ regroups a set of methods to compute derivative information of a function including an optimization problem. If we consider a generic optimization problem parameterized by $(\theta_0, \theta_1, \dots, \theta_m)$:

$$\mathcal{P} : \min_{x} F(x, \theta_0)$$

s.t. $G_i(x, \theta_i) \in S_i \ \forall i \in \{1, \dots, m\}.$

Differentiable optimization in its generic form entails computing the derivative of the output $x^* \in \operatorname{argmin}_x \mathcal{P}$ with respect to all parameters, i.e., computing the Jacobian matrix:

$$\frac{\partial x^*}{\partial \theta} \equiv \left(\frac{\partial x_j^*}{\partial \theta_i}\right)_{ij}$$

Instead of the Jacobian matrix of the *solution map*, $\psi(\theta) = x^*$, we often reason on the the derivative of the solution map as a linear map denoted as $D\psi(\theta)$, with adjoint $D^T\psi(x)$. In general, the solution map is not smooth, it is even a set-valued map and not a simple function from parameters to solution. Some lines of work have investigated non-smooth automatic (sub)differentiation and the behaviour of automatic differentiation in the non-smooth case [Kakade and Lee, 2018, Bolte and Pauwels, 2020]. However, in most cases in differentiable programming, a heuristic quantity is computed when the limit of the directional derivative is ill-defined¹. The recent survey [Kotary et al., 2021] on learning with constrained optimization offers a review of $\partial \mathcal{O}$ techniques. We briefly go over the lines of work that are closest to the methods implemented in DiffOpt.jl.

A part of the recent work on ∂O has focused on specific optimization problems. In [Blondel et al., 2020], the authors consider a differentiable optimization method for sorting and ranking problems. In [Berthet et al., 2020], the differentiation of the solution to a generic convex optimization problem with respect to a linear objective is considered. When the feasible set is a polytope, the issue of a Jacobian matrix being zero almost everywhere arises similarly to the ranking problem from [Blondel et al., 2020]. The approach followed is that of perturbed optimization, considering the input cost vector as a random variable centered around a nominal value. This allows sampling the output solution and Jacobian matrix from input cost vectors generated from the distribution, yielding unbiased estimators for both while only requiring access to a linear minimization oracle i.e. duality information is not required.

For differentiation with respect to arbitrary problem parameters, two main methods have recently appeared in the literature. The first method, from [Amos and Kolter, 2019], can be applied to convex quadratic optimization problems while the second, from [Agrawal et al., 2020], is applied to conic optimization problems. Both methods are based on rewriting necessary optimality conditions for the optimization problem as a system of non-linear equations and then applying the Implicit Function Theorem [Dontchev and Rockafellar, 2009].

^{1.} See the ChainRules.jl recommendations https://juliadiff.org/ChainRulesCore.jl/ v1.14/maths/nondiff_points.html, accessed April 2022

A major step towards integrating differentiable optimization into ML pipelines was presented in [Amos and Kolter, 2019, Amos, 2019] for convex quadratic problems (QP). The considered optimization models are of the form:

$$\min_{x \in \mathbb{R}^n} x^T Q x + c^T x$$
$$G x \le h : (\lambda)$$
$$A x = b : (\mu)$$

where $\lambda \in R^p$, $\mu \in R^m$ denote the dual variables associated with the inequality, equality constraints respectively. Unlike prior work, the solution map is differentiated with respect to all problem data ($A \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^m, G \in \mathbb{R}^{p \times n}, h \in \mathbb{R}^p, Q \in \mathbb{R}^{n \times n}, c \in \mathbb{R}^n$). In particular, differentiating the solution with respect to constraint coefficients opens new applications including learning the constraints of the convex problem along with solutions as illustrated in [Amos, 2019] on generic polytopes and Sudoku problems. The solution method consists in representing the solution process as solving a system of equations. The solution can then be differentiated with respect to its parameters using implicit differentiation. In the case of QPs, the KKT conditions of the system fully describe the optimality conditions for a primal-dual solution:

$$Qx + c + A^{T}\mu + G^{T}\lambda = 0 \qquad (\nabla L)$$

$$Ax = b \qquad (P_{eq})$$

$$0 \le h - Gx \perp \lambda \ge 0 \qquad (C),$$

where (∇L) represents the gradient of the Lagrangian, (P_{eq}) represents the primal feasibility of equality constraints and (C) includes primal feasibility of inequality constraints, complementarity and dual feasibility for inequalities. A system of necessary equality constraints can be derived:

$$(\nabla L), \ (P_{eq}),$$

 $\lambda_i(h - Gx)_i = 0 \ \forall i$

This representation can be implicitly differentiated:

$$dQx + Qdx + dc + dA^{T}\mu + A^{T}d\mu + dG^{T}\lambda + G^{T}d\lambda = 0$$

$$dAx + Adx - db = 0$$

$$d\lambda_{i}(h - Gx)_{i} + \lambda_{i}(dh - dGx - Gdx)_{i} = 0 \quad \forall i.$$

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Regrouping the differential forms of parameters and solution variables results in the following system:

$$\begin{bmatrix} Q & G^T & A^T \\ D(\lambda)G & D(h-Gx) & 0 \\ A & 0 & 0 \end{bmatrix} \begin{bmatrix} dx \\ d\lambda \\ d\mu \end{bmatrix} = -\begin{bmatrix} dQ x + dc + dG^T\lambda + dA^T\mu \\ D(\lambda)dh - D(\lambda)dG x \\ dAx - db \end{bmatrix}$$

where $D(\cdot)$ denotes the diagonal matrix formed from a given vector. The system above can be used to compute several quantities of interest. At a given point

$$(\theta = (c, Q, A, G, b, h), x, \lambda, \mu),$$

solving the system can let us derive the full Jacobian matrix. As pointed out in [Amos, 2019], the highly sparse structure of the matrix on the right-hand side can be exploited to compute some partial derivatives first by selecting only some rows, which are then back-substituted. However, in most applications where derivative information is needed, we only need to perform Jacobian-vector products (JVP) or vector-transpose-Jacobian products (VJP), thus exposing the two principal modes of differentiation present in differentiable libraries or Automatic Differentiation (AD) tools: forward- and reverse-mode AD.

Although QPs capture numerous problems of interest, many problems require a richer set of constraints which can be modelled as conic constraints. Convex conic optimization problems have standard closed-form primal and dual expressions,

Primal Problem	Dual Probler	n
$\min_{x\in R^n} c^T x$	$\min_{y\in R^m}$	$b^T y$
s.t. $Ax + s =$	b s.t.	$A^T y + c = 0$
$s \in \mathcal{K}$		$y \in \mathcal{K}^*$

where *x* is the primal variable, *y* is the dual variable, $s \in \mathbb{R}^m$ is the primal slack variable, $\mathcal{K} \subseteq \mathbb{R}^m$ is a closed convex cone and $\mathcal{K}^* \subseteq \mathbb{R}^m$ is the corresponding dual cone. Note that in above form, $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$, $c \in \mathbb{R}^n$ are problem data.

The methodology of ∂O has been developed for conic problems in [Amos, 2019] and [Agrawal et al., 2020] in parallel and extended in [Agrawal et al., 2019]. The conic case is more involved due to the conic constraints, we follow closely the notation of [Agrawal et al., 2020] for a complete and self-contained description of the method. Instead of deriving the necessary system of equations from the KKT conditions, the proposed approach will rely on the Homogeneous Self-Dual Embedding (HSDE) [O'Donoghue et al., 2016]. In this case the solution map from the problem data to the primal dual pair, $(x, y, s) = \psi(A, b, c)$, is represented as a composition of three functions: $\psi = \phi \circ S \circ Q$. The definition of each of these functions and their derivatives are given by:

1. *Q* maps the problem data, (A, b, c) to the a skew-symmetric matrix $Q \in \mathbb{R}^{n+m+1}$:

$$Q = \begin{bmatrix} 0 & A^T & c \\ -A & 0 & b \\ -c^T & -b^T & 0 \end{bmatrix}, \text{ and its differential is: } dQ = \begin{bmatrix} 0 & dA^T & dc \\ -dA & 0 & db \\ -dc^T & -db^T & 0 \end{bmatrix}$$

2. *S* maps the *Q* matrix from the HSDE into its solution z = (u, v, w). In order to compute the derivative of this function, the author [Agrawal et al., 2020] use the normalized residual map, defined in [Busseti et al., 2019]:

$$\mathcal{N}(z,Q) = ((Q-I)\Pi + I)\left(\frac{z}{|z_{n+m+1}|}\right),$$

where Π is the projection operator onto the Cartesian product $\mathbb{R}^n \times \mathcal{K}^* \times \mathbb{R}_+$. They key point is that, given a matrix Q, the solution z of $\mathcal{N}(z, Q) = 0$ is the solution of the HSDE. Hence,

it is possible to implicitly differentiate the equation $\mathcal{N}(S(Q), Q) = 0$ and obtain:

$$DS(Q) = -(D_z \mathcal{N}(S(Q), Q))^{-1} D_Q \mathcal{N}(S(Q), Q),$$

where

$$D_{Q}\mathcal{N}(z,Q)[U] = U\Pi(\frac{z}{z_{n+m+1}})$$

$$D_{z}\mathcal{N}(z,Q) = \frac{((Q-I)D\Pi(z)+I)}{z_{n+m+1}} - \operatorname{sign}(z_{n+m+1})((Q-I)\Pi+I)(\frac{z}{z_{n+m+1}^{2}})e_{n+m+1}^{T}$$

where $D_x f(x, y)[v]$ denotes the directional derivative of f at x in direction v and e_{n+m+1} the basis vector with 1 at index n + m + 1. Note that the second term of $D_z \mathcal{N}(z, Q)$ vanishes if z is a solution of the HSDE.

3. ϕ maps the solution of the HSDE to the primal-dual pair:

$$(x, y, s) = \phi(z) = \phi(u, v, w) = (u, \Pi_{\mathcal{K}^*}(v), \Pi_{\mathcal{K}^*}(v) - v)/z_{n+m+1}.$$

Its derivative is given by:

$$D\phi(z) = \begin{bmatrix} I & 0 & -x \\ 0 & D\Pi_{\mathcal{K}^{*}}(v) & -y \\ 0 & D\Pi_{\mathcal{K}^{*}}(v) - I & s \end{bmatrix}$$

The derivatives of projections onto classic cones like the positive orthant, second-order, positive semidefinite, and exponential cones are given in [Busseti et al., 2019] and implemented for DiffOpt in MathOptSetDistances.jl[Besançon et al., 2022]. Exponential cone projections are performed using the technique from [Friberg, 2021].

The methodology of differentiable conic problems has been extended to log-log convex problems in [Agrawal and Boyd, 2020], using the grammar from Disciplined Geometric Programming and the rules established for parameterized disciplined convex problems in [Agrawal et al., 2019]. A differentiable method has been developed for submodular functions in [Djolonga and Krause, 2018], opening ∂O to optimization problems with discrete structures. In [Gould et al., 2019], deep learning models are studied with nonlinear optimization problems as nodes instead of closed-form functions, defining a differentiable optimization method for nonlinear problems without requiring convexity. The authors leverage implicit differentiation of the Lagrangian reformulation at the optimal point to estimate derivative information of the output solution with respect to input parameters of the node.

The framework proposed in [Paulus et al., 2021] extends ∂O to optimization problems including integer constraints. Similar to previous work in the convex setting and unlike prior models tackling combinatorial problems, their method handles the differentiation of constraints using an estimation of active constraints at the optimum in the backpropagation phase. In [Blondel et al., 2021], differentiable optimization is viewed as a problem of implicit differentiation. By expressing the solution map of the optimization problem as the root of a system of equation (such as the KKT conditions) or the solution to a fixed point equation, the system can leverage automatic differentiation (AD) of the implicit equations to differentiate the solution map. The approach generalizes the differentiation of quadratic and conic optimization from [Amos and Kolter, 2019] and [Agrawal et al., 2019] but requires a user-defined system of equations that are necessary for optimality.

3. Package structure

DiffOpt is a Julia package that offers differentiable optimization algorithms to the JuMP ecosystem. In order to integrate seamlessly with other packages, DiffOpt is built on top of MathOptInterface.jl (MOI), a foundational unifying package for constrained optimization, designed to be a backend for modelling interfaces such as JuMP.jl or Convex.jl. MOI allows the user to describe structured optimization problems in a unified format based on the constraint representation of functions of variables belonging to sets. This abstraction covers a wide variety of problems including linear, quadratic, and conic constraints as well as more specific sets, such as Special Ordered Sets or complementarity constraints. Moreover, MOI includes a *bridging* mechanism turning the user-provided problem into a problem structure that the chosen solver accepts through successive transformations (or bridges) of the function-set pairs.

The design of MOI enables extending its interface though various mechanisms. First, constraints are defined as pairs func-in-set where func is a function of the decision variables and set is a set in which the value of the function should belong when evaluated at feasible points. Solvers that can exploit special problem structure can therefore allow the user to communicate it by defining new function or set types.

Second, most of the MOI interface is built on top of *attributes*. This enables both the user to communicate custom information to the solver such as starting values or callbacks but also the solver to communicate custom results such as basis status for simplex solvers or Irreducible Inconsistent Subsystems (IIS) for infeasible instances.

Third, MOI optimizers support a layered structure to combine several features. These layers also supports custom constraints and attributes that are typically defined by an inner layer thanks to the well-posed API of MOI. These layers are commonly referred to as *meta-solvers* as they form solvers parameterized by other solvers. Bridges are defined as MOI layers that transform constraints into constraints of different types for its inner layer. When defining a new constraint type, defining bridges to transform it into classical constraint types allows the user to encode this special structure in models while still being able to use solvers not supporting this structure. Below are a few examples of MOI extensions that illustrate this.

SumOfSquares.jl defines the Sum-of-Squares cone as a new set type [Weisser et al., 2019] and *Gram matrices*, *Moment matrices* and *Sum-of-Squares decompositions* as new attributes. It then defines a bridge for transforming Sum-of-Squares constraints into semidefinite constraints. The bridges is applied for all semidefinite programming solvers except for the solver Hypatia.jl [Coey et al., 2020] which supports this custom structure.

Dualization.jl [Bodin et al., 2021] offers a dualization meta-solver. The optimization problem is automatically converted to its dual form and reaches the internal solver only in dual form, of which the solution is then mapped back to the user.

Other extensions have been developed, like QuadraticToBinary.jl [Garcia, 2021], another meta-solver that converts quadratically-constrained problems into Mixed Integer Linear Programs. Also, constraint programming solvers have defined new sets and functions [Kröger, 2020].

DiffOpt can be decomposed into 5 components and aspects that are covered in the following five sections. First, it extends MOI by creating new attributes allowing the user and solver to communicate forward or reverse differentiation input and output. Second, it implements the quadratic and conic problem differentiation rules described in Section 2 as MOI models implementing these attributes. Third, it implements the communication of these attributes through the MOI caching and bridging layers. Fourth, it implements a meta-solver that implements the computation of the differentiation attributes and is parametrized by a solver that should support solving the problem. Fifth, it allows to integrate optimization layers into AD systems in Julia using the ChainRulesCore.jl package.

3.1 Interface

After the problem is solved, the user can pass parameter perturbations in case of forward differentiation or sensitivities with respect to solution variable values in the case of reverse differentiation (or even both). These are passed to the DiffOpt.Optimizer using the attributes detailed in Table 1. After sensitivities are loaded, the user might call DiffOpt.forward_differentiate! or DiffOpt.reverse_differentiate! to compute the derivatives with respect to the input sensitivities. The resulting derivatives are queried again as typical solver attributes, detailed in Table 2.

ForwardObjectiveFunction	Forward-mode tangent for the objective function
ForwardConstraintFunction	Forward-mode tangent for a constraint function
ReverseVariablePrimal	Reverse-mode tangent for a variable value

Table 1: Differential Optimization attributes (DiffOpt attributes for short) for passing per-
turbations and sensitivities.

ForwardVariablePrimal	Forward-mode tangent for a variable value
ReverseObjectiveFunction	Reverse-mode tangent for the objective function
ReverseConstraintFunction	Reverse-mode tangent for a constraint function

 Table 2: Differential Optimization attributes (DiffOpt attributes for short) for querying resulting derivatives.

Perturbations are passed and queried in form of MOI functions (affine functions and quadratic functions) associated with constraints or the objective. The coefficients of vari-

ables (or quadratic terms) are the perturbations related to those variables (or quadratic terms) and the respective associated constraint or objective. This API allows the perturbation to flow through model transformations defined by the above mentioned *bridges*. To keep the API efficient the returned functions are lazily computed so that the only the coefficients required by the final user are actually evaluated.

DiffOpt integrates smoothly with JuMP just like any solver implementing the MOI interface. Because derivative-related attributes are slightly more complex than traditional attributes, JuMP was added as a dependency so that we could overload a small subset of the JuMP API to achieve a better use experience. Moreover, DiffOpt can communicate with any solver that has an MOI interface, more than 30 of them are listed in the JuMP Manual [JuMP Developers, 2021].

3.2 Differentiation rules as MOI models

DiffOpt implements the differentiation rules for QPs (resp. CPs) described in Section 2 as a *differentiation optimization MOI model* (*DiffOpt model* for short) QuadraticDiffProblem (resp. ConicDiffProblem). These DiffOpt models represent QPs (resp. CPs) in the matrix standard form described in Section 2. They do not support solving the QP (resp. CP) but they support having the primal and dual solution being set by the user. Then, they support the differentiation API described in Section 3.1.

The QP and CP standard forms described in Section 2 seems quite restrictive. For inthe QP form supports inequality constraints Gxstance, \leq h, i.e., MOI.ScalarAffineFunction-in-MOI.LessThan, but not Gx h. ≥ i.e., MOI.ScalarAffineFunction-in-MOI.GreaterThan,. This requires the user to transform their model in order to fit the solver-compatible representation. It is then quite tedious and error-prone to map both the primal and dual solutions through these transformations as well as the DiffOpt attributes. Fortunately, as described in the next section, the transformation of these attributes through bridges is implemented. Therefore, adding a bridging outer-layer on top of DiffOpt.QuadraticDiffProblem or DiffOpt.ConicDiffProblem allows the user to model the QP or CP in the most convenient form while all these transformations are carried out transparently. Moreover, it also allows extending DiffOpt to new problem classes through bridges. For instance, as SumOfSquares.jl defines the transformation from a Sum-of-Squares constraint to a semidefinite constraint using a bridge, defining how to transform the DiffOpt attributes through these bridges automatically broadens the class of programs supported by DiffOpt.ConicDiffProblem to Sum-of-Squares programs.

3.3 Model transformations

Most model transformations rely in an affine relation between two sets $S_1 \subseteq \mathbb{R}^n$, S_2 of the form

$$S_1 = \{ x \in \mathbb{R}^n \mid \exists u \in \mathbb{R}^m \text{ s.t. } Ax + Bu + c \in S_2 \}.$$

In fact, at the time of writing, the only bridge in MOI not based on such relation is the bridge from a convex quadratic constraint to a rotated second order cone constraint as it relies on the Cholesky decomposition which is not a linear map.

As detailed in [Legat, 2020, Section 2.1.2], there is an automated way to implement the transformation for primal and dual results given the transformation data A, B and c. Similarly, we develop in this section the transformation for the DiffOpt attributes.

Given a constraint $f_1(x) \in S_1$, the bridges transforms it into a constraint $f_2(x, u) \in S_2$ by adding variables $u \in \mathbb{R}^m$ where $f_2(x, u) = Af_1(x) + Bu + c$. We have $df_2 = A df_1$. Therefore, we see that, the ForwardConstraintFunction forward-mode tangent Δf_1 should be mapped to $A\Delta f_1$ and the ReverseConstraintFunction reverse-mode tangent Δf_2 should be mapped to $A^*\Delta f_2$, with A^* the adjoint matrix of A satisfying

$$\langle Ax, y \rangle_2 = \langle x, A^*y \rangle_1$$

for all *x* in the space of S_1 and *y* in the dual space of S_2 where $\langle \cdot, \cdot \rangle_i$ is the scalar product between the space of S_i and its dual space for i = 1, 2.

3.4 Meta-solver

DiffOpt is designed as a meta-solver with a structure illustrated in Figure 1. The main structure made available by the package is DiffOpt.Optimizer that is parametrized by a mathematical programming inner solver. This inner solver may be any object supporting storing and solving the problem provided by the user. As shown in Figure 1, the entry point is a cache that is added to ensure efficient storage and access of the user model. Also, bridge layers are added as the user model may use constraint types that are not natively supported by the inner solver (or the DiffOpt models) and need to be transformed. The solution found by the inner solver is communicated to the DiffOpt model as described in Section 3.2. This model is then used to compute forward and/or reverse differentiation tangents.

Note that the bridges used for the inner solver and for the DiffOpt model are completely independent. They can be entirely different as the primal and dual results are automatically transformed through the inner solver bridge layer from the solver solution into the solution corresponding to the user model and then through the DiffOpt model bridges into the solution corresponding to the DiffOpt model standard form.

This design of DiffOpt.Optimizer also enables adding new DiffOpt models in addition to DiffOpt.QuadraticProgram.Model and DiffOpt.ConicProgram. Model in order to further broaden the class of supported model.



Figure 1: Design of the DiffOpt.Optimizer structure

Because MOI does not differentiate between the two considered classes QP and CP, the user can pass any of the two problem classes to DiffOpt without ever having to know which of the two methods will be used. DiffOpt automatically selects the appropriate problem class based on the type of constraints and objective function.

In the following code excerpt, we demonstrate the usage of DiffOpt, starting from a simple JuMP model, then going through a reverse differentiation procedure.

```
using JuMP, DiffOpt, Clp
model = JuMP.Model(() -> diff_optimizer(Clp.Optimizer))
@variable(model, x)
(constraint(model, cons, x \ge 3))
@objective(
   model,
   Min,
   2x,
)
optimize! (model) # solve
MOI.set.( # set pertubations / gradient inputs
   model,
    DiffOpt.ReverseVariablePrimal(),
   х,
   1.0,
)
DiffOpt.reverse_differentiate!(model) # differentiate
# fetch expression of the gradient of constraint
grad\_exp = MOI.get( \# -3x+1)
   model.
   DiffOpt.ReverseConstraintFunction(),
   cons
)
JuMP.constant(grad_exp) # 1
JuMP.coefficient(grad_exp, x) \# -3
```

3.5 ChainRules integration

Automatic Differentiation (AD) has become a cornerstone of machine learning, evolving from the static transformation of program sources to a fully dynamic process [Innes et al., 2019]. The Julia AD landscape has been evolving rapidly [Schäfer et al., 2021] and is now converging towards a shared set of derivative primitives implemented for elementary functions and exploited by AD libraries to compute derivatives of full programs. The methods to implement to provide derivative information are defined in ChainRulesCore.jl [JuliaDiff, 2021] and implemented in ChainRules.jl for Julia Base and standard library functions.

One drawback is that the ChainRules.jl system reasons on the differentiation of a function's output with respect to its inputs. The DiffOpt interface however is based on MOI and thus on the incremental construction of a model represented as a single mutable object. One approach is to construct an implementation of the solution map which takes as argument the model parameters, builds and optimizes the model object, and returns the optimal solution. The solution map is a pure function and its derivatives can be expressed in terms of ChainRules.jl primitives and implemented using derivative information from DiffOpt.

The implementation allows external users to effortlessly bring any MOI model built directly or through a modelling interface like JuMP or Convex.jl to a differentiable pipeline, regardless of the underlying solver used to solve the main model. However, the user still needs to write down the solution map and implement the ChainRules.jl interface functions frule and rrule for forward and reverse differentiation respectively. We will demonstrate how DiffOpt and ChainRules.jl can be combined in the following section.

4. Application examples

We discuss how differentiating an optimization program allows a variety of applications for different computational tasks. These examples use various convex solvers to compute the primal and dual solutions, in order to highlight the ease to swap a solver for another in a single line.

All the following examples can be seen in detail in the *Tutorials* section of the DiffOpt manual. The code and data use version 0.4 of the package.

4.1 Sensitivity Analysis

Sensitivity analysis [Saltelli et al., 2004] focuses on studying how the changes in the inputs of a mathematical model affects its output. Sensitivities of a JuMP model can be computed automatically using the previously described methods. We illustrate sensitivity analysis for a classification and a regression task.

4.1.1 Classification using SVM

Support vector machines (SVM) classify labelled data points with the hyperplane minimizing the norm of classification errors on all points (or achieve the largest margin if the two classes are separable). Assuming $X \in \mathbb{R}^{n \times d}$ the feature matrix of *n* data points with *d* features and *y* their labels, a soft-margin ℓ_1 -SVM with ℓ_2 regularization can be modelled as:

$$\min_{\substack{\xi, w, b \\ \xi_i = 1}} \sum_{i=1}^n \xi_i + \lambda \|w\|^2$$

s.t. $y_i(w^T X_i + b) \ge 1 - \xi_i \quad \forall i \in 1..n$
 $\xi_i \ge 0 \quad \forall i \in 1..n,$

where e_i is the soft margin loss on the i - th data point, $w^T x = b$ is the SVM hyperplane, λ is the regularization parameter.

The plots and code transcripts are from *Sensitivity Analysis of SVM* tutorial. The model is implemented below and solved using Ipopt [Wächter and Biegler, 2006].

```
# N, D, X, y are given

λ = 0.05

model = Model(() -> DiffOpt.diff_optimizer(Ipopt.Optimizer))

# Add the variables
```

Using the forward differentiation mode of DiffOpt, we compute the partial Jacobian with respect to each *i*-th individual data point and display its norm:

$$\left\|\frac{\partial w}{\partial X_i}\right\| + \left|\frac{\partial b}{\partial X_i}\right|.$$

The computation is performed as follows:

```
v = zeros(N)
for i in 1:N
   for j in 1:N
       if i == j
           # identical perturbations on all x_i
            MOI.set(
               model,
               DiffOpt.ForwardConstraintFunction(),
               con[j],
                y[j] * sum(w),
            )
        else
            MOI.set(
               model,
                DiffOpt.ForwardConstraintFunction(),
                con[j],
                0.0,
            )
        end
    end
    DiffOpt.forward_differentiate!(model)
    dw = MOI.get.(
       model,
       DiffOpt.ForwardVariablePrimal(),
        w,
    )
    db = MOI.get(
       model,
       DiffOpt.ForwardVariablePrimal(),
       b,
    )
    v[i] = norm(dw) + norm(db)
end
```

A perturbation of the feature matrix X affects the solution and can induce a change in the separating hyperplane decisions (w, b). Unlike other classification models, not



Figure 2: Learned SVM and sensitivities. Data points colors indicate the class and marker size denoting the sensitivity of the hyperplane to x_i .

all points affect the hyperplane with small enough perturbations, the optimal solution depends only on a few data points, the support vectors that name the method. The impact of these perturbations are displayed in Figure 2.

4.1.2 Ridge regression sensitivity

Ridge regression avoids overfitting with an ℓ_2 -norm penalty added to a linear regression model and is particularly advantageous when the number of features is as large as the number of observations. Assume $X = \{(x, y)\} \subset \mathbb{R}^{d+1}$ to be the set of *n* data points. Then a ridge regression fitting problem can be modelled as:

$$\min_{w,b} \quad \sum_{i=1}^{N} (y_i - w^T x_i - b)^2 + \alpha (\|w\|_2^2 + b^2)$$

with α the regularization constant.

The plots and code transcripts are from *Sensitivity Analysis of Ridge Regression* tutorial. We implement and solve below a univariate example with DiffOpt using Ipopt as the underlying QP solver.

```
# X, Y, N are given
model = Model(() -> diff_optimizer(Ipopt.Optimizer))
@variable(model, w)
@variable(model, b)
alpha = 0.8  # regularization constant
@expression(model, e[i=1:N], Y[i] - w * X[i] - b)
@objective(
```

```
model,
Min,
1 / N * dot(e, e) + alpha * (w^2 + b^2),
)
optimize!(model)
```

Similar to the SVM example, a change in a single independent or dependent variable value x_i or y_i for a given data point can affect the learned model. We use DiffOpt in forward mode to quantify these sensitivities to individual data points:

$$\frac{\partial w}{\partial x_i}$$
 and $\frac{\partial w}{\partial y_i}$.

A ForwardInObjective attribute can be set for the perturbation of the objective function. It takes as input the expression proportionally dependent on the perturbed parameter θ . Given a generic expression $f(x; \theta) = \theta g(x)$ with parameter θ , the expected input is g(x). A particular aspect here is that the x_i and y_i values appear as linear and quadratic term in the loss function. If the parameter θ appears both linearly and quadratically, the corresponding objective perturbation can be derived with a first-order Taylor expansion:

$$\begin{split} f(x;\theta) &= \theta g(x) + \theta^2 h(x) \\ f(x;\theta+\delta) &= (\theta+\delta)g(x) + \theta^2 h(x) + 2\delta\theta h(x) + \delta^2 h(x) \\ f(x;\theta+\delta) &\approx f(x;\theta) + \delta(g(x) + 2\theta h(x)). \end{split}$$

When applied to the loss function, the perturbation $\delta_i^{(x)}$, $\delta_i^{(y)}$ on x_i , y_i respectively results in first-order perturbation approximations:

$$\delta_i^{(x)}(2w^2x_i + 2bw - 2wy_i),$$

 $\delta_i^{(y)}(2y_i - 2b - 2wx_i)$

respectively. Using these input perturbations we can extract the output sensitivity of the slope *w* using the DiffOpt.ForwardOutVariablePrimal variable attribute:



Figure 3: Sensitivity analysis of the data points in ridge regression. Radius of the markers is proportional to the sensitivity of the slope to x or y perturbations. Blue markers indicate a negative sensitivity, red markers a positive one.

```
MOI.set(
    model,
    DiffOpt.ForwardObjectiveFunction(),
    (2Y[i] - 2b - 2w * X[i]),
)
DiffOpt.forward_differentiate!(model)
    vy[i] = MOI.get(model, DiffOpt.ForwardOutVariablePrimal(), w)
end
```

Figure 3 shows how sensitive in amplitude and direction is the slope *w* to perturbations of each data point.

4.2 Convex Optimization for Neural Network Layers

Most of the common neural network layers are either simple closed-form operators or a composition of several operators. ∂O opens new possibilities by providing derivatives for layers defined as solutions to optimization problems. The derivatives computed by DiffOpt can be used to backpropagate through the convex layer.

4.2.1 CUSTOM RELU LAYER

This example will follow the tutorial Custom ReLU layer of the documentation.

The Rectified Linear Unit or ReLU, a commonly used linear layer in machine learning networks, is defined as $f(x) = \max\{x, 0\}$. It can be interpreted as projecting a point $x \in \mathbb{R}^n$ onto the non-negative orthant.

$$\min_{y \ge 0} \|x - y\|_2^2$$

where y is the optimization variable and x is the output.

Using the above definition, we model ReLU as a layer in a neural network created in Flux.jl [Innes, 2018]. The model was trained on MNIST image dataset [LeCun et al., 2010]

with 60,000 greyscale training bitmaps of size 28×28. We define the function matrix_relu with a matrix input because it allows training in batches, the first dimension of the matrix is the layer size, while the second dimension is the size of the batch.

```
function matrix_relu(
    y::Matrix;
    model = Model(() -> DiffOpt.diff_optimizer(Ipopt.Optimizer))
)
    layer_size, batch_size = size(y)
    empty!(model)
    set_silent(model)
    @variable(model, x[1:layer_size, 1:batch_size] >= 0)
    @objective(model, Min, x[:]'x[:] -2y[:]'x[:])
    optimize!(model)
    return value.(x)
end
```

Using our function as a neural network layer requires a corresponding derivative implementation to differentiate the model and propagate the gradients backward. This can be achieved using DiffOpt in conjunction with ChainRules by defining a method for the reverse-mode primitive function rrule.

```
function ChainRulesCore.rrule(::typeof(matrix_relu), y::Matrix{T}) where T
   model = Model(() -> DiffOpt.diff_optimizer(Ipopt.Optimizer))
   pv = matrix_relu(y, model = model)
   function pullback_matrix_relu(dl_dx)
      x = model[:x] # load decision variable `x` into scope
       dl_dy = zeros(T, size(dl_dx))
       dl_dq = zeros(T, size(dl_dx))
        # set sensitivities
       MOI.set.(model, DiffOpt.ReverseVariablePrimal(), x[:], dl_dx[:])
        # compute grad
       DiffOpt.reverse_differentiate!(model)
       # return gradient wrt objective parameters
       obj_exp = MOI.get(model, DiffOpt.ReverseObjectiveFunction())
       # coeff of `x` in q'x = -2y'x
       dl_dq[:] .= JuMP.coefficient.(obj_exp, x[:])
       dq_dy = -2 # dq/dy = -2
       dl_dy[:] .= dl_dq[:] * dq_dy
       return (ChainRulesCore.NoTangent(), dl_dy)
   and
   return pv, pullback_matrix_relu
end
```

Note the ChainRulesCore.NoTangent term which corresponds to the derivative of the output with respect to the function matrix_relu itself. The next example will demonstrate how to handle stateful functions. Since this is a pure function, no derivative is defined. We can now define the neural network architecture including our custom layer and train it on the MNIST data.

```
using MLDatasets
using Flux
```

```
# neural network definition
layer size = 10
m = Flux.Chain(
    Flux.Dense(784, layer_size), # 784 being image linear dimension (28 x 28)
    matrix relu,
    Flux.Dense(layer_size, 10), # 10 being the number of outcomes (0 to 9)
    Flux.softmax,
)
# dataset preprocessing
N = 1000 \# batch size
imgs = MLDatasets.MNIST.traintensor(1:N)
labels = MLDatasets.MNIST.trainlabels(1:N)
train_X = float.(reshape(imgs, size(imgs, 1) * size(imgs, 2), N))
train_Y = Flux.onehotbatch(labels, 0:9);
epochs = 50
dataset = repeated((train_X, train_Y), epochs)
# neural network optimization
custom_loss(x, y) = crossentropy(m(x), y)
opt = Flux.ADAM()
Flux.train!(custom_loss, params(m), dataset, opt)
```

Implementing a custom layer for a known closed-form function is not directly useful, and solving a quadratic problem is costly in contrast with a simple ReLU operation. However, it opens the door to more flexible variations of the layer.

4.2.2 POLYHEDRAL PROJECTION LAYER

We generalize the custom layer defined as an optimization problem from the ReLU example. This use case is available in the tutorials as *Polyhedral QP layer*.

Given *m* vector-scalar pairs $(w_i, b_i) \forall i \in 1..m$, we define the layer taking *y* as input and projecting it on the polytope defined by the *m* hyperplanes:

$$\begin{aligned} \min_{x} \|x - y\|_{2}^{2} \\
\text{s.t. } w_{i}^{T} x \ge b_{i} \quad \forall i \in 1..m
\end{aligned}$$

Instead of a function, we will represent the layer with a functor (or callable object).

```
struct Polytope{N}
w::NTuple{N, Vector{Float64}}
b::Vector{Float64}
end
Polytope(w::NTuple{N}) where {N} = Polytope{N}(w, randn(N))
```

We define a "call" operation on the polytope, making it a so-called functor. Calling the polytope with a matrix y operates an Euclidean projection of each of the matrix columns onto the polytope.

```
function (polytope::Polytope{N}) (
    y::AbstractMatrix;
    model = direct_model(DiffOpt.diff_optimizer(Ipopt.Optimizer))
) where {N}
```

```
layer_size, batch_size = size(y)
empty!(model)
set_silent(model)
@variable(model, x[1:layer_size, 1:batch_size])
@constraint(model,
    greater_than_cons[idx in 1:N, sample in 1:batch_size],
    dot(polytope.w[idx], x[:, sample]) ≥ polytope.b[idx]
)
@objective(model, Min, dot(x - y, x - y))
optimize!(model)
return JuMP.value.(x)
end
Flux.@functor Polytope
```

The @functor macro from Flux implements auxiliary functions for collecting the parameters of our custom layer and operating backpropagation. Similarly to the ReLU example, ChainRulesCore.rrule is used to implement the reverse-mode differentiation of the layer.

```
function ChainRulesCore.rrule(
       polytope::Polytope{N},
       y::AbstractMatrix) where {N}
   model = direct_model(DiffOpt.diff_optimizer(Ipopt.Optimizer))
   xv = polytope(y; model = model)
   function pullback(dl_dx)
       layer_size, batch_size = size(dl_dx)
       dl_dx = ChainRulesCore.unthunk(dl_dx)
       # `dl_dy` is the derivative of `l` wrt `y`
       x = model[:x]
        # grad wrt input parameters
       dl_dy = zeros(size(dl_dx))
        # grad wrt layer parameters
       dl_dw = zero.(polytope.w)
       dl_db = zero(polytope.b)
       # set sensitivities
       MOI.set.(model, DiffOpt.ReverseVariablePrimal(), x, dl_dx)
        # compute grad
       DiffOpt.reverse_differentiate!(model)
        # compute gradient wrt objective function parameter y
       obj_expr = MOI.get(model, DiffOpt.ReverseObjectiveFunction())
       dl_dy .= -2 * JuMP.coefficient.(obj_expr, x)
       greater_than_cons = model[:greater_than_cons]
        for idx in 1:N, sample in 1:batch_size
            cons_expr = MOI.get(model,
               DiffOpt.ReverseConstraintFunction(),
               greater_than_cons[idx, sample])
            dl_db[idx] -= JuMP.constant(cons_expr)/batch_size
            dl_dw[idx] .+= JuMP.coefficient.(cons_expr, x[:,sample])/batch_size
        end
       dself = ChainRulesCore.Tangent{Polytope{N}} (; w = dl_dw, b = dl_db)
       return (dself, dl_dy)
   end
   return xv, pullback
end
```

Note that the inner pullback returns a ChainRulesCore.Tangent that represents the tangent of a composite type. This will allow Flux to operate gradient descent on the parameters of the Polytope struct directly. Similarly to the previous example, we can now build and train the network (we omit other details like dataset preprocessing):

```
layer_size = 20
m = Flux.Chain(
    Flux.Dense(784, layer_size), # 784 being image linear dimension (28 x 28)
    Polytope((randn(layer_size), randn(layer_size), randn(layer_size))),
    Flux.Dense(layer_size, 10), # 10 being the number of outcomes (0 to 9)
    Flux.softmax,
)
Flux.train!(custom_loss, Flux.params(m), dataset, opt)
```

The capacity to embed a convex problem as a neural network layer enables formulations of SVMs or regression layers with custom constraints which have direct applications in meta-learning [Lee et al., 2019].

4.3 Hyperparameter optimization

Most machine learning algorithms involve hyperparameters that require tuning to accelerate the training process and reach good out-of-sample performance, helping achieve balance between model variance and bias. In the past few years, many developments were made in gradient-based methods [Maclaurin et al., 2015] where researchers typically introduced extra hyperparameters for tuning. Recent interest in automated machine learning (AutoML) has resulted in a resurgence of research in this field [Feurer and Hutter, 2019].

When the learning process can be formulated as solving an optimization problem of which the hyperparameters are parameters, the problem of out-of-sample optimization can be formulated as a bilevel optimization problem [Guyon et al., 2019]:

$$\min_{\theta} f(X_{test}, \hat{w}, \theta)$$

s.t. $\hat{w} \in \operatorname*{argmin}_{w} f(X_{train}, w, \theta),$

with w the learned weights of the prediction model, $X_{train/test}$ the training and testing data, f the loss function and θ the hyperparameter. Depending on the expression of $\nabla_{\theta} f(\cdot, \cdot, \cdot)$, computing (even local) optima of the bilevel optimization problem can be challenging. We showcase how DiffOpt can be used to meta-optimize the weights and the hyperparameters following the DiffOpt tutorial *Auto-tuning Hyperparameters*.

4.3.1 Optimization problem

Let $X = \{(x, y) | x \in \mathbb{R}^d, y \in \mathbb{R}\}$ be the set of *N* data points of dimension *D*. The regularized linear model can be modelled as an optimization problem of the form:

$$\min_{w} \quad \frac{1}{2nD} \sum_{i=1}^{n} (y_i - w^T x_i)^2 + \frac{\alpha}{2D} \|w\|_2^2 \tag{1}$$

where $w \in \mathbb{R}^D$ are the learned weights and α , the regularization parameter, is the only hyperparameter. Since the problem is strongly convex, it admits a unique minimum w^* . Its implementation in JuMP is given below.

```
import JuMP
function fit_ridge(model, X, y, a)
   JuMP.empty!(model)
   set_silent(model)
   N, D = size(X)
   @variable(model, w[1:D])
   @expression(model, err_term, X * w - y)
   @objective(
        model,
        Min,
        dot(err_term, err_term) / (2 * N * D) + a * dot(w, w) / (2 * D),
   )
   optimize!(model)
   return w
end
```

4.3.2 Model differentiation

We want to find the optimal regularization parameter for the loss on a test set that was not used to find the optimal weights. We will apply gradient descent of the unregularized test loss with respect to α , for which we need to compute its gradient $\frac{\partial l}{\partial \alpha}$. This can be achieved using the chain rule:

$$\frac{\partial l}{\partial \alpha}(w,\alpha) = \nabla_w l(w,\alpha) \frac{\partial w}{\partial \alpha}(w,\alpha)$$

where $\frac{\partial w}{\partial \alpha}$ is the derivative of the optimal solution of Problem (1) w.r.t. the parameter and can be found using DiffOpt as follows:

```
function compute_dw_da(model, w)
   D = length(w)
   dw d\alpha = zeros(D)
    MOI.set(
       model.
       DiffOpt.ForwardObjectiveFunction(),
       dot(w, w) / (2 * D),
    DiffOpt.forward_differentiate!(model)
    for i in 1:D
        dw_d\alpha[i] = MOI.get(
            model,
            DiffOpt.ForwardVariablePrimal(),
            w[i],
        )
    end
    return dw_dα
end
function d_testloss_da(model, X_test, y_test, w, ŵ)
   N, D = size(X_test)
   dw_d\alpha = compute_dw_d\alpha (model, w)
   err_term = X_test * \hat{w} - y_test
    return sum(eachindex(err_term)) do i
       dot(X_test[i,:], dw_da) * err_term[i]
    end / (N * D)
end
```



Figure 4: Mean squared error on the training Figure 5: Gradient descent on the test set for and test set against α a using DiffOpt

4.3.3 Hyperparameter gradient descent

The value of α is updated using a fixed-step gradient descent scheme implemented below:

```
function descent (\alpha0, max_iters=100; fixed_step = 0.01, grad_tol=1e-3)
    \alpha_s = Float64[]
     \partial \alpha_s = \text{Float64[]}
     test_loss = Float64[]
     \alpha = \alpha 0
     N, D = size(X_test)
     model = Model(() -> DiffOpt.diff_optimizer(Ipopt.Optimizer))
     for iter in 1:max_iters
          w = fit_ridge(model, X_train, y_train, \alpha)
          \hat{w} = value.(w)
          err\_term = X\_test * \hat{w} - y\_test
          \partial \alpha = d_{testloss} d\alpha (model, X_{test}, y_{test}, w, \hat{w})
          push! (\alpha_s, \alpha)
          push!(\partial \alpha_s, \partial \alpha)
          push!(test_loss, norm(err_term)^2 / (2 * N * D))
          \alpha -= fixed_step * \partial \alpha
          if abs(\partial \alpha) \leq grad_tol
                break
          end
     end
     return \alpha_s, \partial \alpha_s, test_loss
end
```

4.3.4 NUMERICAL RESULTS

The mean squared error of the regression on the training and test sets is displayed in Figure 4, normalized for display. For values of α below ≈ 0.23 , the model is under-regularized i.e. overfitted to the training data, increasing α improves the test error. After that point, increasing α excessively shrinks the regression coefficients, increasing the error.

Figure 5 displays the trajectory of the gradient descent procedure described in Section 4.3.3, starting from $\alpha_0 = 0.1$ and performing about 120 iterations.

Cross-validation is the typical procedure applied to tune the hyperparameters of learning models. Leveraging ∂O lets us replace black-box optimization procedures that are typical for hyperparameters with any first-order method that leverages the gradient obtained from DiffOpt.

5. Conclusion

DiffOpt allows users to differentiate through optimization problems implementing MathOptInterface, formulated with high-level modelling systems like JuMP or Convex.jl. The package brings a flexible differentiable optimization framework beyond disciplined convex optimization, separating the underlying implementation from the MOI idiomatic interface. This separation of concerns opens the possibility for the integration of novel differentiable optimization techniques for classes of problems not already covered.

Future work will also consider performance improvements. In particular, using DiffOpt to tune hyperparameters or construct a convex optimization layer requires fast computation of derivatives and reoptimization of a perturbed primal problem. The two steps could be integrated to cache more information and reduce the computational burden per iteration.

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