

Efficient and Modular Implicit Differentiation

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Gradient-based learning

- Gradient-based training algorithms are the workhorse of modern machine learning.
- Deriving gradients by hand is tedious and error prone.
- This becomes quickly infeasible for complex models.
- Changes to the model require rederiving the gradient.
- Deep learning = GPU + data + autodiff
- This talk: differentiating optimization problem solutions

Outline

1 Automatic differentiation

2 Argmin differentiation

3 Proposed framework

4 Experimental results

Automatic differentiation

- Evaluates the derivatives of a function at a given point.
- Not the same as numerical differentiation.
- Not the same as symbolic differentiation, which returns a "human-readable" expression.
- In a neural network context, reverse autodiff is often known as backpropagation.

Automatic differentiation

- A program is defined as the composition of primitive operations that we know how to derive.
- The user can focus on the forward computation / model.

```
import jax.numpy as jnp
from jax import grad, jit
```

```
def predict(params, inputs):
    for W, b in params:
        outputs = jnp.dot(inputs, W) + b
        inputs = jnp.tanh(outputs)
    return outputs
```

```
def logprob_fun(params, inputs, targets):
    preds = predict(params, inputs)
    return jnp.sum((preds - targets)**2)
```

```
grad_fun = jit(grad(logprob_fun))
```

Automatic differentiation

Modern frameworks support higher-order derivatives

```
def tanh(x):
 y = jnp.exp(-2.0 * x)
 return (1.0 - y) / (1.0 + y)
fp = grad(tanh)
fpp = grad(grad(tanh))
```

Forward-mode vs. Reverse-mode

Forward-mode

- Computes Jacobian vector products (JVPs) along the forward pass
- Each JVP call builds one column of the Jacobian
- Efficient for tall Jacobians (more outputs than inputs)
- Need not store intermediate computations

Reverse-mode

- Computes vector Jacobian products (VJPs) in reverse order
- Each VJP call builds one row of the Jacobian
- Efficient for wide matrices (more inputs than outputs)
- Needs to store intermediate computations

Key components of an autodiff system

- JVPs and/or VJPs for all primitive operations
- Obtaining the computational graph
 - Ahead of time (from source or using a DSL)
 - Just in time (graph is built while being executed)
- Topological sort
- Forward-mode: forward pass (JVPs)
- Reverse-mode: forward pass + backward pass (VJPs)





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Notation

Small letters for scalar-valued functions, e.g., f

• The gradient of $f: \mathbb{R}^d \to \mathbb{R}$

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(\mathbf{x}) \\ \vdots \\ \frac{\partial f}{\partial x_d}(\mathbf{x}) \end{bmatrix} \in \mathbb{R}^d$$

• The Hessian of $f : \mathbb{R}^d \to \mathbb{R}$ evaluated at $x \in \mathbb{R}^d$

$$\nabla^2 f(x) = \begin{bmatrix} \frac{\partial^2 f(x)}{\partial x_1^2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_d \partial x_1} & \cdots & \frac{\partial^2 f(x)}{\partial x_d^2} \end{bmatrix} \in \mathbb{R}^{d \times d}$$

Notation

- Capital letters for vector-valued functions, e.g., F
- The Jacobian of $F : \mathbb{R}^d \to \mathbb{R}^p$ evaluated at $x \in \mathbb{R}^d$

$$\partial F(x) = \begin{bmatrix} \frac{\partial F_1(x)}{\partial x_1} & \cdots & \frac{\partial F_1(x)}{\partial x_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial F_p(x)}{\partial x_1} & \cdots & \frac{\partial F_p(x)}{\partial x_d} \end{bmatrix} = \begin{bmatrix} \nabla F_1(x)^\top \\ \vdots \\ \nabla F_p(x)^\top \end{bmatrix} \in \mathbb{R}^{p \times d}$$

■ Jacobian-vector product (JVP) with $u \in \mathbb{R}^d$

 $\partial F(x)u \in \mathbb{R}^p$

Vector-Jacobian product (VJP) with $v^{\top} \in \mathbb{R}^{p}$

$$v^{\top}\partial F(x) \in \mathbb{R}^d$$

Argmin differentiation

Consider the optimization

$$x^{\star}(\theta) = \operatorname*{argmin}_{x \in \mathbb{R}^d} f(x, \theta)$$

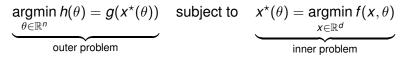
where $f: \mathbb{R}^d \times \mathbb{R}^n \to \mathbb{R}$ is twice differentiable

• $x^* : \mathbb{R}^n \to \mathbb{R}^d$ is an implicit function

- Extensions: constrained optimization, non-smooth optimization
- How to compute the Jacobian $\partial x^{\star}(\theta) \in \mathbb{R}^{d \times n}$?
- Autodiff cannot be used as is: $x^{\star}(\theta)$ has no closed form in general

Argmin differentiation

Application 1: bi-level optimization



Gradient of the outer problem: $\nabla h(\theta) = \partial x^{\star}(\theta)^{\top} \nabla g(x^{\star}(\theta))$

Useful in hyperparam optimization, meta-learning

Application 2: "optimization as a layer"

$$\cdots \rightarrow x^{\star}(\theta) \rightarrow \ldots$$

Can impose structure on the output via regularization or constraints

Application 3: sensitivity analysis; ∂x*(θ) may be interesting in its own right (e.g., to answer a scientific question)

Unrolling

Consider the sequence produced by an iterative algorithm

```
x_0(\theta), x_1(\theta), \ldots, x_K(\theta)
```

where

$$x_k(\theta) = T(x_{k-1}(\theta), \theta)$$

- If the algorithm is convergent, $\hat{x}(\theta) = x_{\mathcal{K}}(\theta)$ can be used as an approximation of $x^{*}(\theta)$
- Idea: use $\partial \hat{x}(\theta)$ as an approximation of $\partial x^{\star}(\theta)$

Unrolling

Pros

- relatively simple (can use autodiff transparently)
- derivatives $\partial \hat{x}(\theta)$ are consistent with forward pass $\hat{x}(\theta)$

Cons

- must reimplement the algorithm from scratch using the autodiff system (cannot reuse state-of-the-art software)
- not all algorithms are autodiff friendly,
- complexity scales linearly with n (forward-mode)
- memory scales linearly with K (reverse-mode), which is especially problematic on GPU
- the latter can be mitigated by using checkpointing, which trade-offs recomputations for smaller memory requirement

Implicit differentiation

- Use some optimality conditions to mathematically derive an expression of $\partial x^*(\theta)$
- Examples that have been used in the past:
 - Stationary conditions
 - Karush–Kuhn–Tucker (KKT) conditions
 - Proximal gradient fixed point
- Often involves the resolution of a linear system
- So far, the derivation and implementation were case-by-case and sometimes complicated
- Not flexible: modeling changes require rederiving the expression of $\partial x^*(\theta)$

cvxpy layers

- cvxpy: an optimization toolbox for easily formulating convex optimization problems
- Reduces all problems to linear conic programing
- cvxpy layers (Agrawal et al 2019): making cvxpy differentiable
- Uses conic programming optimality conditions to derive a formula of the Jacobian
- Pro: very general (supports any convex problem)
- Con: conic solvers are rarely the state-of-the-art for each specific problem instance







3 Proposed framework

4 Experimental results

Overview

- Makes it very easy to add implicit differentiation on top of any solver (ability to reuse state-of-the-art implementations)
- The user provides (in Python) a mapping F: ℝ^d × ℝⁿ → ℝ^d capturing the optimality conditions solved by the solver
- We combine autodiff of *F* and implicit differentiation to automatically differentiate x^{*}(θ)
- Decouples the implicit differentiation mechanism from the optimality condition speficiation (in previous works, they were intertwined)
- Flexible: no mathematical derivation needed from the user, ability to experiment easily

Example: differentiating ridge regression

```
X_tr, y_tr = load_data()
```

```
def f(x, theta): # objective function
  residual = jnp.dot(X_tr, x) - y_tr
  return (jnp.sum(residual ** 2) + theta * jnp.sum(x ** 2)) / 2
```

F = jax.grad(f) # optimality condition

```
@custom_root(F)
def ridge_solver(theta):
    XX = jnp.dot(X_tr.T, X_tr)
    Xy = jnp.dot(X_tr.T, y_tr)
    I = jnp.eye(X_tr.shape[0])
    return jnp.linalg.solve(XX + theta * I, Xy)
```

```
print(jax.jacobian(ridge_solver)(10.0))
```

Differentiating a root

- Let *F* : ℝ^d × ℝⁿ → ℝ^d be a user-provided mapping, capturing the optimality conditions of a problem
- An optimal solution $x^*(\theta)$ should be a **root** of *F*:

 $F(x^{\star}(\theta), \theta) = 0$

- Implicit function theorem: ∂x*(θ) exists if ∂₁F is a square invertible matrix at (x*(θ), θ)
- Using the chain rule, we get

$$\partial_1 F(x^*(\theta), \theta) \partial x^*(\theta) + \partial_2 F(x^*(\theta), \theta) = 0$$

$$\iff \underbrace{-\partial_1 F(x^*(\theta), \theta)}_{A \in \mathbb{R}^{d \times d}} \underbrace{\partial x^*(\theta)}_{J \in \mathbb{R}^{d \times n}} = \underbrace{\partial_2 F(x^*(\theta), \theta)}_{B \in \mathbb{R}^{d \times n}}$$

Differentiating a fixed point

In many case $x^*(\theta)$ will be a fixed point:

$$x^{\star}(\theta) = T(x^{\star}(\theta), \theta)$$

where $T: \mathbb{R}^d \times \mathbb{R}^n \to \mathbb{R}^d$

This is of course a special case since we can define

$$F(x^{\star}(\theta), \theta) = T(x^{\star}(\theta), \theta) - x^{\star}(\theta) = 0$$

Gradient descent

Let $x^*(\theta)$ be implicitly defined as

$$x^{\star}(\theta) = \operatorname*{argmin}_{x \in \mathbb{R}^d} f(x, \theta),$$

where $f: \mathbb{R}^d \times \mathbb{R}^n \to \mathbb{R}$ is twice differentiable

F is simply the gradient mapping

$$F(x,\theta) = \nabla_1 f(x,\theta)$$

Equivalently, we can use the gradient descent fixed point

$$T(\mathbf{x},\theta) = \mathbf{x} - \eta \nabla_1 f(\mathbf{x},\theta)$$

for any $\eta > 0$

KKT conditions

Consider the problem

 $\operatorname*{argmin}_{z\in\mathbb{R}^{p}}f(z, heta)$ subject to $G(z, heta)\leq0,\ H(z, heta)=0$

where G and H can be vector-valued

The stationarity, primal feasibility and complementary slackness conditions give

$$\nabla_1 f(z, \theta) + [\partial_1 G(z, \theta)]^\top \lambda + [\partial_1 H(z, \theta)]^\top \nu = 0$$
$$H(z, \theta) = 0$$
$$\lambda \circ G(z, \theta) = 0$$

where $\nu \in \mathbb{R}^q$ and $\lambda \in \mathbb{R}^r_+$ are the dual variables

This can be written as $F(x^*(\theta), \theta) = 0$ if we denote $x^*(\theta) = (z^*(\theta), \nu^*(\theta), \lambda^*(\theta))$

KKT conditions

```
In code:
```

```
grad = jax.grad(f)
def F(x, theta):
  z, nu, lambd = x
  theta_f, theta_H, theta_G = theta
  _, H_v_{jp} = jax_v_{jp}(H, z, theta_H)
  stationarity = (grad(z, theta_f) + H_v jp(nu)[0])
 primal_feasability = H(z, theta_H)
  _, G_vjp = jax.vjp(G, z, theta_G)
  stationarity += G_vjp(lambd)[0]
  comp_slackness = G(z, theta_G) * lambd
```

return stationarity, primal_feasability, comp_slackness

Quadratic programming

Consider the QP

$$\underset{z \in \mathbb{R}^{p}}{\operatorname{argmin}} f(z, \theta) = \frac{1}{2} z^{\top} Q z + c^{\top} z \quad \text{s.t.} \quad H(z, \theta) = E z - d = 0,$$
$$G(z, \theta) = M z - h \le 0.$$

The KKT conditions for this QP can again be written as F(x*(θ), θ) = 0 if we write

$$\begin{aligned} x^{\star}(\theta) &= (z^{\star}(\theta), \nu^{\star}(\theta), \lambda^{\star}(\theta)) \\ \theta &= (Q, c, E, d, M, h) \end{aligned}$$

Just need to express *f*, *H* and *G* directly in Python

Proximal gradient fixed point

Let $x^{\star}(\theta)$ be implicitly defined as

$$x^{\star}(heta)\coloneqq rgmin_{x\in\mathbb{R}^d} f(x, heta)+g(x, heta)$$

where $g \colon \mathbb{R}^d \times \mathbb{R}^n \to \mathbb{R}$ is potentially non-smooth

We can use the proximal gradient fixed point

$$T(x,\theta) = \operatorname{prox}_{\eta g}(x - \eta \nabla_1 f(x,\theta), \theta)$$

where we defined the proximity operator

$$\operatorname{prox}_{g}(y,\theta) \coloneqq \operatorname*{argmin}_{x \in \mathbb{R}^{d}} \frac{1}{2} \|x - y\|_{2}^{2} + g(x,\theta)$$

- Proximal operators are Lipschitz continuous and therefore differentiable almost everywhere
- Many enjoy a closed-form (soft thresholding, block soft thresholding, ...)

Proximal gradient fixed point

In code:

```
grad = jax.grad(f)
def T(x, theta):
   theta_f, theta_g = theta
   return prox(x - grad(x, theta_f), theta_g)
```

Projected gradient fixed point

Let $x^{\star}(\theta)$ be implicitly defined as

$$x^{\star}(\theta) = \operatorname*{argmin}_{x \in \mathcal{C}(\theta)} f(x, \theta)$$

where $C(\theta)$ is a convex set depending on θ

We can use the projected gradient fixed point

$$T(x, \theta) = \operatorname{proj}_{\mathcal{C}}(x - \eta \nabla_1 f(x, \theta), \theta)$$

where we defined the Euclidean projection operator

$$\operatorname{proj}_{\mathcal{C}}(y,\theta) \coloneqq \operatorname*{argmin}_{x \in \mathcal{C}(\theta)} \|x - y\|_2^2$$

Our library provides plenty of reusable projections

Summary of optimality mappings

Name	Solution needed	ed Oracles needed	
Stationary	Primal	$\nabla_1 f$	
KKT	Primal and dual	$\nabla_1 f, H, G, \partial_1 H, \partial_1 G$	
Proximal gradient	Primal	$\nabla_1 f$, prox _{ng}	
Projected gradient	Primal	$\nabla_1 f$, proj _C	
Mirror descent	Primal	$\nabla_1 f$, proj ^{φ} , $\nabla \varphi$	
Newton	Primal	$[\nabla_1^2 f(x,\theta)]^{-1}, \nabla_1 f(x,\theta)$	
Block proximal gradient	Primal	$[\nabla_1 f]_j$, $[\operatorname{prox}_{\eta g}]_j$	
Conic programming	Residual map root	$proj_{\mathbb{R}^{p} imes \mathcal{K}^{*} imes \mathbb{R}_{+}}$	

Oracles are accessed through their JVP or VJP.

Computing JVPs and VJPs

Integrating $x^*(\theta)$ in forward-mode autodiff requires JVPs

To obtain the JVP Ju, solve

$$A(Ju) = Bu$$

Integrating $x^*(\theta)$ in reverse-mode autodiff requires VJPs

To obtain the VJP $v^{\top}J$, solve

$$A^{\top}u = v$$

then

$$v^{\top}J = u^{\top}AJ = u^{\top}B$$

Solving the linear systems

- When A is positive semi-definite, we can use conjugate gradient
- When A is indefinite, we can use GMRES or BiCGSTAB
- All algorithms only require access to A or A^T through matrix-vector products (linear maps)
- Since $A = \partial_1 F$ and $B = \partial_2 F$, we only access to JVPs or VJPs of F
- When A is indefinite, an alternative is the normal equation

$$A^{\top}AJ = A^{\top}B$$

which can be solved using conjugate gradient

Features needed from an autodiff system

JVPs and VJPs

- Second derivatives when *F* includes the gradient mapping $\nabla_1 f(x, \theta)$
- Custom JVPs and VJPs: this is how we are able to create @custom_root and @custom_fixed_point
- jax.vmap: vectorizing map (automatic batching)
- jax.linear_transpose: automatic transposition of linear maps

Jacobian bounds

In practice, we almost never get $x^*(\theta)$ and thus never solve

$$\underbrace{-\partial_1 F(x^*(\theta), \theta)}_{A \in \mathbb{R}^{d \times d}} \underbrace{\partial x^*(\theta)}_{J \in \mathbb{R}^{d \times n}} = \underbrace{\partial_2 F(x^*(\theta), \theta)}_{B \in \mathbb{R}^{d \times n}}$$

Let $J(\hat{x}, \theta)$ be the solution of the linear system at \hat{x} instead of $x^*(\theta)$

• Under regularity conditions on $\partial_1 F$ and $\partial_2 F$, we can show (Thm 1)

$$\|J(\hat{x}, heta) - J(x^{\star}(heta), heta)\| = \|J(\hat{x}, heta) - \partial x^{\star}(heta)\| < \mathcal{C}\|\hat{x} - x^{\star}(heta)\|$$

i.e., J is Lipschitz

We then apply this result to the (proximal) gradient descent fixed point under regularity conditions directly on *f* and prox_g (cf. corollaries 1 and 2)





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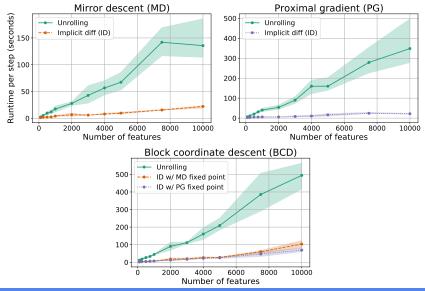
Hyperparam optim of multiclass SVMs

- Goal: find hyperparameters that perform well on validation data
- $x^{\star}(\theta) \in \mathbb{R}^{m \times k}$: optimal dual variables
- $\theta \in \mathbb{R}_+$: regularization parameter
- bi-level optimization problem

$$\underbrace{\min_{\theta = \exp(\lambda)} \frac{1}{2} \| X_{\text{val}} W(x^{\star}(\theta), \theta) - Y_{\text{val}} \|_{F}^{2}}_{\text{outer problem}} \quad \text{s.t.} \quad \underbrace{x^{\star}(\theta) = \underset{x \in \mathcal{C}}{\operatorname{argmin}} \frac{\theta}{2} \| W(x, \theta) \|_{F}^{2}}_{\text{inner problem}}$$

$$\begin{split} \mathcal{C} &\coloneqq \bigtriangleup^k \times \ldots \bigtriangleup^k \\ W(x, \theta) &\coloneqq X_{\text{tr}}^\top (Y_{\text{tr}} - x) / \theta \in \mathbb{R}^{p \times k} \end{split}$$

Hyperparam optim of multiclass SVMs



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Hyperparam optim of multiclass SVMs

```
X tr. Y tr. X val. Y val = load data()
def W(x. theta): # dual-primal map
  return jnp.dot(X_tr.T, Y_tr - x) / theta
def f(x, theta): # inner objective
  return 0.5 * theta * jnp.sum(W(x, theta) ** 2)
grad = jax.grad(f)
proj = jax.vmap(projection_simplex)
def T(x, theta):
  return proj(x - grad(x, theta))
@custom fixed point(T)
def msvm dual solver(theta):
  # [...7
  return x_star # solution of the dual objective
def outer_loss(lambd):
  theta = inp.exp(lambd)
  x star = msvm dual solver(theta) # inner solution
  Y_pred = jnp.dot(W(x_star, theta), X_val)
  return 0.5 * jnp.sum((Y_pred - Y_val) ** 2)
```

```
print(jax.grad(outer_loss)(lambd))
```

Task-driven dictionary learning

- Goal: breast cancer survival prediction from gene expression data
- $x^{\star}(\theta) \in \mathbb{R}^{m \times k}$: sparse codes (atom weights for each sample)
- $\theta \in \mathbb{R}^{k \times p}$: dictionary of k atoms
- bi-level optimization problem

$$\underbrace{\min_{\theta \in \mathbb{R}^{k \times p}, w \in \mathbb{R}^{k}, b \in \mathbb{R}} \sigma(x^{\star}(\theta)w + b; y_{tr})}_{\text{outer problem}} \quad \text{s.t.} \quad x^{\star}(\theta) \in \underset{x \in \mathbb{R}^{m \times k}}{\operatorname{argmin} f(x, \theta) + g(x)}_{\text{inner problem}}$$

where

 $f(x, \theta) := \ell(X_{tr}, x\theta)$: data reconstruction error σ : binary logistic loss

Task-driven dictionary learning

Method L ₁ logreg	L ₂ logreg	DictL + L_2 logreg	Task-driven DictL
AUC (%) 71.6 ± 2.0	$\textbf{72.4} \pm \textbf{2.8}$	68.3 ± 2.3	$\textbf{73.2} \pm \textbf{2.1}$

- binary classification problem to discriminate patients who survive longer than 5 years ($m_1 = 200$) vs patients who die within 5 years of diagnosis ($m_0 = 99$) from p = 1,000 gene expression values
- Performs better than using the original features with 100 fewer variables

Task-driven dictionary learning

```
X_tr, y_tr = load_data()
def f(x. theta): # dictionary loss
  residual = X_tr - jnp.dot(x, theta)
  return huber_loss(residual)
grad = jax.grad(f)
def T(x, theta): # proximal gradient fixed point
  return prox_lasso(x - grad(x, theta))
@custom_fixed_point(T)
def sparse_coding(theta): # inner objective
  # [...]
  return x_star # lasso solution
def outer_loss(theta, w): # task-driven loss
  x_star = sparse_coding(theta) # sparse codes
  y_pred = jnp.dot(x_star, w)
  return logloss(y_tr, y_pred)
```

```
print(jax.grad(outer_loss, argnums=(0,1)))
```

Dataset distillation

- Goal: learn a small "distilled" datataset such that a model trained on this data performs well on the original data
- $x^*(\theta) \in \mathbb{R}^{p \times k}$: logistic regression weights
- $\theta \in \mathbb{R}^{k \times p}$: distilled images ("class prototypes")
- bi-level optimization problem

$$\underbrace{\min_{\theta \in \mathbb{R}^{k \times p}} f(x^{\star}(\theta), X_{\text{tr}}; y_{\text{tr}})}_{\text{outer problem}} \quad \text{s.t.} \quad x^{\star}(\theta) \in \underbrace{\operatorname*{argmin}_{x \in \mathbb{R}^{p \times k}} f(x, \theta; [k]) + \varepsilon \|x\|^2}_{\text{inner problem}}$$

where

$$f(W, X; y) := \ell(y, XW)$$

 ℓ : multiclass logistic loss

Dataset distillation (MNIST)

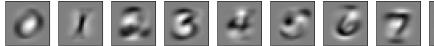
Via implicit diff

Dataset Distillation (MNIST). Generalization Accuracy: 0.8556



Via unrolling (4x slower)

Dataset Distillation (MNIST). Generalization Accuracy: 0.8556



Dataset distillation

```
X_tr, y_tr = load_data()
```

```
logloss = jax.vmap(loss.multiclass_logistic_loss)
```

```
def f(x, theta, l2reg=1e-3): # inner objective
  scores = jnp.dot(theta, x)
 distilled_labels = jnp.arange(10)
 penalty = 12reg * jnp.sum(x * x)
 return jnp.mean(logloss(distilled_labels, scores)) + penalty
```

```
F = iax.grad(f)
```

```
Qcustom root(F)
def logreg_solver(theta):
 # [...]
 return x star
```

```
def outer loss(theta):
 x_star = logreg_solver(theta) # inner solution
 scores = jnp.dot(X_tr, x_star)
 return jnp.mean(logloss(y_tr, scores))
```

```
print(jax.grad(outer_loss)(theta))
```

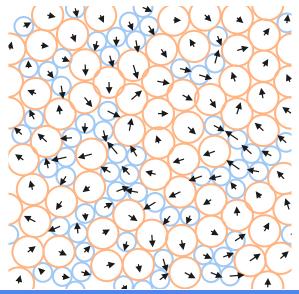
Molecular dynamics

- Goal: sensitivity analysis of molecular dynamics
- $x^*(\theta) \in \mathbb{R}^{k \times 2}$: coordinates of k particles
- $\theta \in \mathbb{R}_+$: diameter of small particles
- optimization problem

$$x^{*}(\theta) = \operatorname*{argmin}_{x \in \mathbb{R}^{k \times m}} f(x, \theta) \coloneqq \sum_{i,j} U(x_{i,j}, \theta)$$

where $U(x_{i,j}, \theta)$ is the pairwise potential energy function

Molecular dynamics: $\partial x^{\star}(\theta) \in \mathbb{R}^{k \times 2}$



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Conclusion

- A general framework combining implicit differentiation with autodiff of optimality conditions
- Flexibility to try out ideas easily
- Ability to add implicit differentiation on top of existing solvers
- Arxiv preprint: https://arxiv.org/abs/2105.15183
- Open-source release: coming soon!
- Thank you for your attention!