



Deep Learning with Nontrivial Constraints

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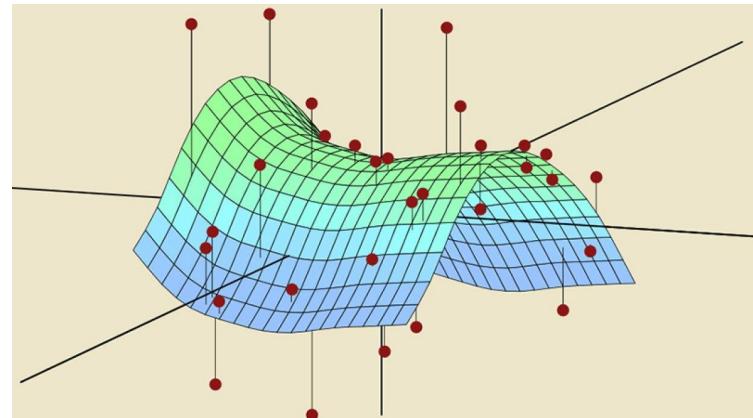
Oct 31, 2025

2025 Annual Midwest Optimization Meeting @ UND



UNIVERSITY OF MINNESOTA
Driven to DiscoverSM

Three fundamental questions in DL



- **Approximation:** is it powerful, i.e., the \mathcal{H} large enough for all possible weights?
- **Optimization:** how to solve
$$\min_{\mathbf{w}'_i s, \mathbf{b}'_i s} \frac{1}{n} \sum_{i=1}^n \ell [\mathbf{y}_i, \{\text{NN}(\mathbf{w}_1, \dots, \mathbf{w}_k, b_1, \dots, b_k)\}(\mathbf{x}_i)]$$
- **Generalization:** does the learned NN work well on “similar” data?

Algorithms

Isn't it solved?

Base class

CLASS `torch.optim.Optimizer(params, defaults)` [source]

Base class for all optimizers.

• WARNING

Parameters need to be specified as collections consistent between runs. Examples of objects and iterators over values of dictionaries.

Parameters:

- **params** (*iterable*) – an iterable of `Tensor`s

Tensors should be optimized.

- **defaults** – (*dict*): a dict containing default values for parameters

when a parameter group doesn't specify them.

`Adadelta`

Implements Adadelta algorithm.

`Adagrad`

Implements Adagrad algorithm.

`Adamax`

Implements Adamax algorithm (a variant of Adam based on infinity norm).

`ASGD`

Implements Averaged Stochastic Gradient Descent.

`LBFGS`

Implements L-BFGS algorithm, heavily inspired by `minFunc`.

`NAdam`

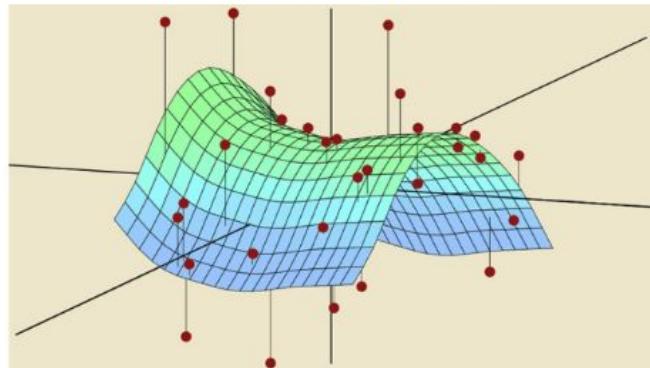
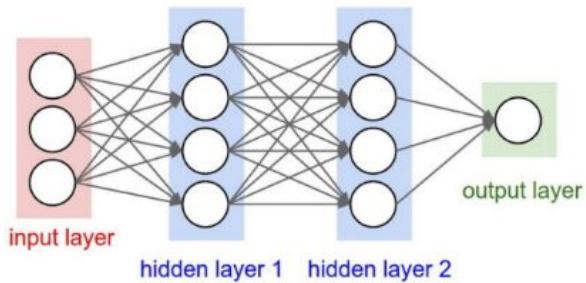
Implements NAdam algorithm.

`RAdam`

Implements RAdam algorithm.

When DL meets constraints

Artificial neural networks



used to approximate nonlinear functions

Unconstrained optimization

$$\min_{\boldsymbol{w}'_i s, \boldsymbol{b}'_i s} \frac{1}{n} \sum_{i=1}^n \ell [y_i, \{\text{NN}(\boldsymbol{w}_1, \dots, \boldsymbol{w}_k, \boldsymbol{b}_1, \dots, \boldsymbol{b}_k)\}(\boldsymbol{x}_i)]$$
$$\min_{\boldsymbol{x}} f(\boldsymbol{x})$$

“Solved”

Constrained optimization

$$\min_{\boldsymbol{x}} f(\boldsymbol{x}) \quad \text{s. t. } g(\boldsymbol{x}) \leq 0$$

largely “unsolved”

This talk is about GAPS

$$\min_{\mathbf{x}} f(\mathbf{x}) \quad \text{s. t. } g(\mathbf{x}) \leq 0$$

largely “unsolved”



An imaginary chat between a PhD student working in deep learning (**DLP**) and a PhD student working in optimization (**OP**)

DLP: Man, I've solved a constrained DL problem recently

OP: Oh, that's a hard problem

DLP: Really? I actually did it

OP: How?

DLP: My problem is $\min_x f(x)$, s.t. $g(x) \leq 0$. I put $g(x)$ as a penalty and then call ADAM

OP: Are you sure it works?

DLP: Yes, the performance is improved and my paper is published at ICML

OP: Why don't you try augmented Lagrangian methods?

DLP: No implementation in Pytorch. Is it possible we work out some theory about my method?

OP: I think it's hard. It's not convex

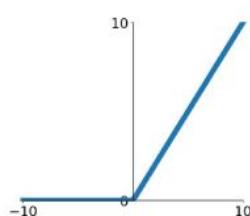
Outline

Constrained deep learning: CDL

- **What, how, and why for CDL**
- No good solvers for CDL yet
- Granso and PyGranso
- PyGranso in action
- Outlook

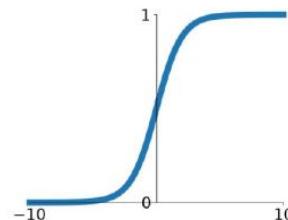
DL with simple constraints

Embedding constraints into DL models



ReLU
(Rectified Linear Unit)

Nonnegativity



Sigmoid

[0, 1]

$$z \mapsto \left[\frac{e^{z_1}}{\sum_j e^{z_j}}, \dots, \frac{e^{z_p}}{\sum_j e^{z_j}} \right]^\top$$

Softmax

Nonnegativity and summed to 1

DL with nontrivial constraints

- Robustness evaluation
- Imbalanced learning
- Topology optimization
- Contrastive learning

Navigation: Home | About | Contact | Log In

Deep Learning with Nontrivial Constraints: Methods and Applications

Chuan He¹, Ryan Devera¹, Wenjie Zhang¹, Ying Cui², Zhaosong Lu³ and Ju Sun¹

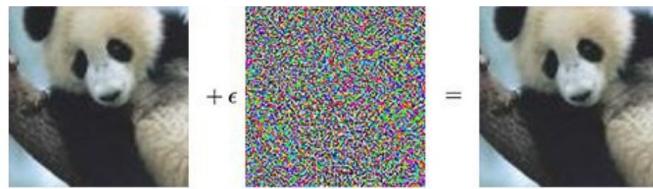
¹Computer Science and Engineering, University of Minnesota

²Industrial Engineering and Operations Research, University of California, Berkeley

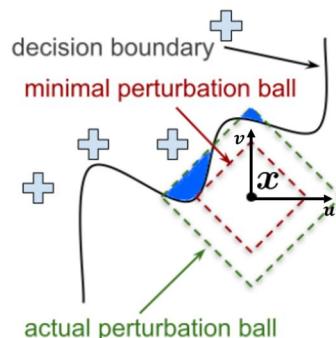
³Industrial and Systems Engineering, University of Minnesota

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Robustness evaluation (RE)



$$\mathbf{x} + \delta = \mathbf{x}'$$



Maximize loss function

$$\max_{\mathbf{x}'} \ell(\mathbf{y}, f_{\boldsymbol{\theta}}(\mathbf{x}'))$$

s. t. $d(\mathbf{x}, \mathbf{x}') \leq \varepsilon$, $\mathbf{x}' \in [0, 1]^n$

Allowable perturbation Valid image

Minimize robustness radius

$$\min_{\mathbf{x}'} d(\mathbf{x}, \mathbf{x}')$$

s. t. $\max_{i \neq y} f_{\boldsymbol{\theta}}^i(\mathbf{x}') \geq f_{\boldsymbol{\theta}}^y(\mathbf{x}')$, $\mathbf{x}' \in [0, 1]^n$

Change the predicted class Valid image

Projected gradient descent (PGD) for RE

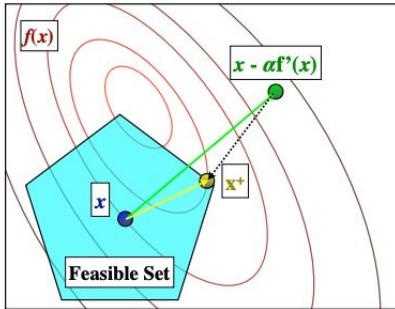
$$\min_{\mathbf{x} \in \mathcal{Q}} f(\mathbf{x})$$

Step size

$$\mathbf{x}_{k+1} = P_{\mathcal{Q}} \left(\mathbf{x}_k - \alpha_k \nabla f(\mathbf{x}_k) \right)$$

$$P_{\mathcal{Q}}(\mathbf{x}_0) = \arg \min_{\mathbf{x} \in \mathcal{Q}} \frac{1}{2} \|\mathbf{x} - \mathbf{x}_0\|_2^2$$

Projection operator



Key hyperparameters:
 (1) step size
 (2) iteration number

$$\max_{\mathbf{x}'} \ell(\mathbf{y}, f_{\theta}(\mathbf{x}'))$$

s. t. $d(\mathbf{x}, \mathbf{x}') \leq \varepsilon$, $\mathbf{x}' \in [0, 1]^n$

Algorithm 1 APGD

```

1: Input:  $f, S, x^{(0)}, \eta, N_{\text{iter}}, W = \{w_0, \dots, w_n\}$ 
2: Output:  $x_{\max}, f_{\max}$ 
3:  $x^{(1)} \leftarrow P_S(x^{(0)} + \eta \nabla f(x^{(0)}))$ 
4:  $f_{\max} \leftarrow \max\{f(x^{(0)}), f(x^{(1)})\}$ 
5:  $x_{\max} \leftarrow x^{(0)}$  if  $f_{\max} \equiv f(x^{(0)})$  else  $x_{\max} \leftarrow x^{(1)}$ 
6: for  $k = 1$  to  $N_{\text{iter}} - 1$  do
7:    $z^{(k+1)} \leftarrow P_S(x^{(k)} + \eta \nabla f(x^{(k)}))$ 
8:    $x^{(k+1)} \leftarrow P_S \left( x^{(k)} + \alpha(z^{(k+1)} - x^{(k)}) \right.$ 
       $\quad \left. + (1 - \alpha)(x^{(k)} - x^{(k-1)}) \right)$ 
9:   if  $f(x^{(k+1)}) > f_{\max}$  then
10:     $x_{\max} \leftarrow x^{(k+1)}$  and  $f_{\max} \leftarrow f(x^{(k+1)})$ 
11:   end if
12:   if  $k \in W$  then
13:     if Condition 1 or Condition 2 then
14:        $\eta \leftarrow \eta/2$  and  $x^{(k+1)} \leftarrow x_{\max}$ 
15:     end if
16:   end if
17: end for

```

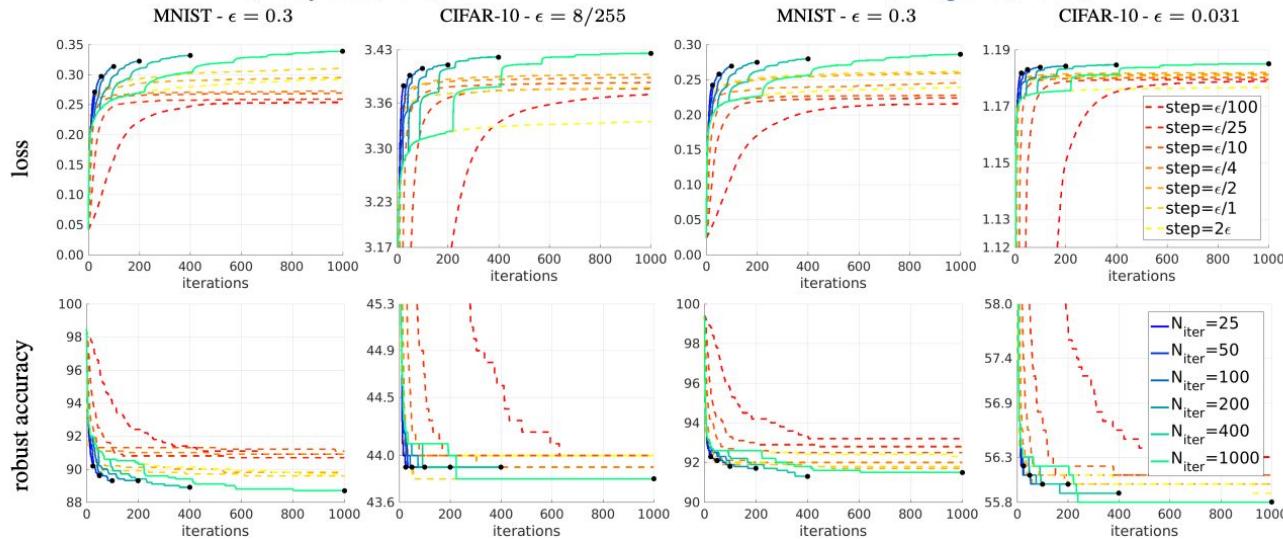
Ref https://angms.science/doc/CVX/CVX_PGD.pdf

<https://www.cs.ubc.ca/~schmidtm/Courses/5XX-S20/S5.pdf>

Reliable evaluation of adversarial robustness with an ensemble of diverse parameter-free attacks. Croce, F., Hein, M., ICML 2020

<https://arxiv.org/pdf/2003.01690.pdf>

Problem with projected gradient descent



$$\max_{\mathbf{x}'} \ell(\mathbf{y}, f_{\boldsymbol{\theta}}(\mathbf{x}'))$$

$$\text{s.t. } d(\mathbf{x}, \mathbf{x}') \leq \varepsilon, \quad \mathbf{x}' \in [0, 1]^n$$

**Tricky to set:
iteration number & step size
i.e., tricky to decide where to stop**

Robustness evaluation: penalty methods for complicated d (perceptual attack)

$$\begin{aligned} & \max_{\mathbf{x}'} \ell(\mathbf{y}, f_{\theta}(\mathbf{x}')) \\ \text{s.t. } & d(\mathbf{x}, \mathbf{x}') \leq \varepsilon, \quad \mathbf{x}' \in [0, 1]^n \end{aligned}$$

$d(\mathbf{x}, \mathbf{x}') \doteq \|\phi(\mathbf{x}) - \phi(\mathbf{x}')\|_2$ **perceptual distance**
 where $\phi(\mathbf{x}) \doteq [\hat{g}_1(\mathbf{x}), \dots, \hat{g}_L(\mathbf{x})]$

Projection onto the constraint is complicated

Penalty methods

$$\max_{\tilde{\mathbf{x}}} \quad \mathcal{L}(f(\tilde{\mathbf{x}}), y) - \lambda \max \left(0, \|\phi(\tilde{\mathbf{x}}) - \phi(\mathbf{x})\|_2 - \epsilon \right)$$

Solve it for each fixed λ and then increase λ

Algorithm 2 Lagrangian Perceptual Attack (LPA)

```

1: procedure LPA(classifier network  $f(\cdot)$ , LPIPS distance  $d(\cdot, \cdot)$ , input  $\mathbf{x}$ , label  $y$ , bound  $\epsilon$ )
2:    $\lambda \leftarrow 0.01$ 
3:    $\tilde{\mathbf{x}} \leftarrow \mathbf{x} + 0.01 * \mathcal{N}(0, 1)$             $\triangleright$  initialize perturbations with random Gaussian noise
4:   for  $i$  in  $1, \dots, S$  do            $\triangleright$  we use  $S = 5$  iterations to search for the best value of  $\lambda$ 
5:     for  $t$  in  $1, \dots, T$  do            $\triangleright T$  is the number of steps
6:        $\Delta \leftarrow \nabla_{\tilde{\mathbf{x}}} [\mathcal{L}(f(\tilde{\mathbf{x}}), y) - \lambda \max(0, d(\tilde{\mathbf{x}}, \mathbf{x}) - \epsilon)]$             $\triangleright$  take the gradient of (5)
7:        $\hat{\Delta} = \Delta / \|\Delta\|_2$             $\triangleright$  normalize the gradient
8:        $\eta = \epsilon * (0.1)^{t/T}$             $\triangleright$  the step size  $\eta$  decays exponentially
9:        $m \leftarrow d(\tilde{\mathbf{x}}, \tilde{\mathbf{x}} + h\hat{\Delta})/h$             $\triangleright m \approx$  derivative of  $d(\tilde{\mathbf{x}}, \cdot)$  in the direction of  $\hat{\Delta}$ ;  $h = 0.1$ 
10:       $\tilde{\mathbf{x}} \leftarrow \tilde{\mathbf{x}} + (\eta/m)\hat{\Delta}$             $\triangleright$  take a step of size  $\eta$  in LPIPS distance
11:    end for
12:    if  $d(\tilde{\mathbf{x}}, \mathbf{x}) > \epsilon$  then
13:       $\lambda \leftarrow 10\lambda$             $\triangleright$  increase  $\lambda$  if the attack goes outside the bound
14:    end if
15:  end for
16:   $\tilde{\mathbf{x}} \leftarrow \text{PROJECT}(d, \tilde{\mathbf{x}}, \mathbf{x}, \epsilon)$ 
17:  return  $\tilde{\mathbf{x}}$ 
18: end procedure

```

Problem with penalty methods

Method	cross-entropy loss		margin loss	
	Viol. (%) ↓	Att. Succ. (%) ↑	Viol. (%) ↓	Att. Succ. (%) ↑
Fast-LPA	73.8	3.54	41.6	56.8
LPA	0.00	80.5	0.00	97.0
PPGD	5.44	25.5	0.00	38.5
PWCF (ours)	0.62	93.6	0.00	100

LPA, Fast-LPA: penalty methods

PPGD: Projected gradient descent

Penalty methods tend to encounter

large constraint violation (i.e., infeasible solution, known in optimization theory) or **suboptimal solution**

$$\begin{aligned} & \max_{\mathbf{x}'} \ell(\mathbf{y}, f_{\theta}(\mathbf{x}')) \\ \text{s.t. } & d(\mathbf{x}, \mathbf{x}') \leq \varepsilon, \quad \mathbf{x}' \in [0, 1]^n \\ & d(\mathbf{x}, \mathbf{x}') \doteq \|\phi(\mathbf{x}) - \phi(\mathbf{x}')\|_2 \end{aligned}$$

where $\phi(\mathbf{x}) \doteq [\hat{g}_1(\mathbf{x}), \dots, \hat{g}_L(\mathbf{x})]$

PWCF, an optimizer with a principled stopping criterion on **stationarity & feasibility**

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DL frameworks



JAX: Autograd and XLA



For unconstrained DL problems

Convex optimization solvers and frameworks



Modeling languages



SDPT³ - a M_{ATLAB} software package for
semidefinite-quadratic-linear programming

[K. C. Toh](#), [R. H. Tütüncü](#), and [M. J. Todd](#).

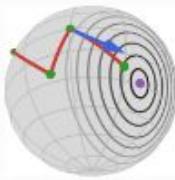
TFOCS: Templates for First-Order Conic Solvers

Solvers

Not for DL, which involves NCVX optimization

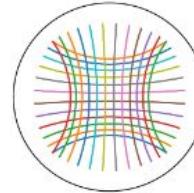
Note: Gurobi can handle certain NCVX problems

Manifold optimization



Manopt.jl

Geomstats



$\mathcal{T}_p \mathcal{G}$
geoopt

McTorch Lib, a manifold optimization library for deep learning

Only for **differentiable manifolds constraints**

General constrained optimization

KNITRO®

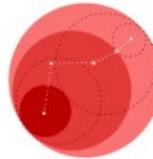


IPOPT

Interior-point methods



Cooper



ensmallen

flexible C++ library for efficient numerical optimization

GENO

Augmented Lagrangian methods

Lagrangian-method-based constrained optimization

TensorFlow Constrained Optimization (TFCO)

Specialized ML packages



Problem-specific solvers that **cannot be easily extended** to new formulations

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Constrained deep learning: CDL

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Issues with typical CDL methods

projected gradient descent

$$\min_{\mathbf{x} \in Q} f(\mathbf{x})$$

$$\mathbf{x}_{k+1} = P_Q \left(\mathbf{x}_k - \alpha_k \nabla f(\mathbf{x}_k) \right)$$

Issue: no principled stopping criterion/step size rules

Lagrangian method

$$\min_{\mathbf{x}} \max_{\lambda \geq 0} \hat{f}(\mathbf{x}) + \lambda^T g(\mathbf{x})$$

Idea: alternating minimize \mathbf{x} and maximize λ via gradient descent

penalty methods

$$\min_{\mathbf{x}} f(\mathbf{x}) \quad \text{s. t. } g(\mathbf{x}) \leq \mathbf{0}$$

$$\min_{\mathbf{x}} f(\mathbf{x}) + \lambda \max(0, g(\mathbf{x}))$$

Solved with increasing λ : sequence

Issue: infeasible solution

Issues

- Infeasible solution
- Slow convergence

Want

- Feasible & stationary solution
- Reasonable speed

Principled answers to these questions

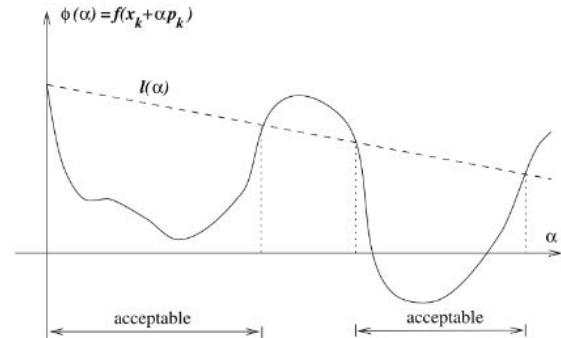
- **Feasible & stationary solution**

Stationarity and feasibility check: KKT condition

- **Reasonable speed**

Line search

- **A hidden problem: nonsmoothness**



Armijo (Sufficient Decrease) Condition



<http://www.timmitchell.com/software/GRANSO/>

Key algorithm

Nonconvex, nonsmooth, constrained

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{x}), \quad \text{s.t. } c_i(\mathbf{x}) \leq 0, \quad \forall i \in \mathcal{I}; \quad c_i(\mathbf{x}) = 0, \quad \forall i \in \mathcal{E}.$$

Penalty sequential quadratic programming (P-SQP)

$$\begin{aligned} \min_{d \in \mathbb{R}^n, s \in \mathbb{R}^p} \quad & \mu(f(x_k) + \nabla f(x_k)^T d) + e^T s + \frac{1}{2} d^T H_k d \\ \text{s.t.} \quad & c(x_k) + \nabla c(x_k)^T d \leq s, \quad s \geq 0, \end{aligned}$$

Ref: **Curtis, Frank E., Tim Mitchell, and Michael L. Overton.** "A BFGS-SQP method for nonsmooth, nonconvex, constrained optimization and its evaluation using relative minimization profiles." *Optimization Methods and Software* 32.1 (2017): 148-181.

Algorithm highlights

Steering strategy for the penalty parameter

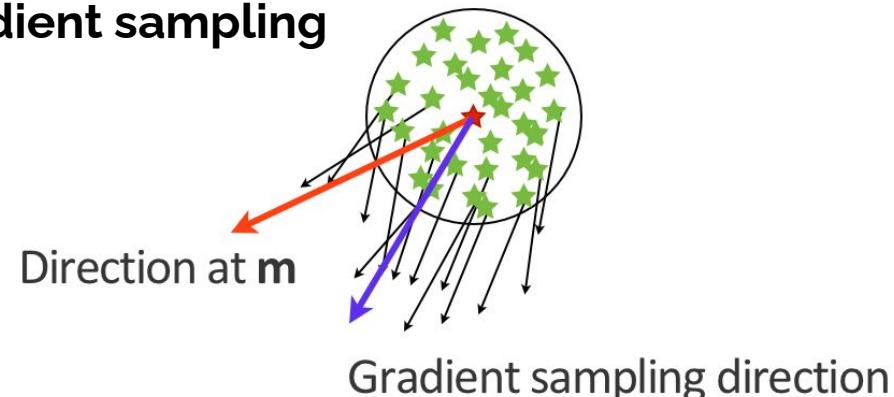
If feasibility improvement is insufficient : $l_\delta(d_k; x_k) < c_v v(x_k)$

Stationarity based on (approximate) gradient sampling

$$G_k := [\nabla f(x^k) \quad \nabla f(x^{k,1}) \quad \cdots \quad \nabla f(x^{k,m})]$$

$$\min_{\lambda \in \mathbb{R}^{m+1}} \frac{1}{2} \|G_k \lambda\|_2^2$$

$$\text{s.t. } \mathbf{1}^T \lambda = 1, \quad \lambda \geq 0$$



Key take-away



- Principled stopping criterion and line search, to obtain a **solution with certificate** (stationarity & feasibility check)
- Quasi-newton style method for fast convergence, i.e.,
reasonable speed and high-precision solution

Ref Curtis, Frank E., Tim Mitchell, and Michael L. Overton. "A BFGS-SQP method for nonsmooth, nonconvex, constrained optimization and its evaluation using relative minimization profiles." Optimization Methods and Software 32.1 (2017): 148-181.



Limitations of GRANSO

```
% Gradient of inner product with respect to A  
f_grad      = imag((conj(Bty)*Cx.')/(y'*x));  
f_grad      = f_grad(:);  
  
% Gradient of inner product with respect to A  
ci_grad     = real((conj(Bty)*Cx.')/(y'*x));  
ci_grad     = ci_grad(:);
```

analytical gradients required

```
p           = size(B,2);  
m           = size(C,1);  
X           = reshape(x,p,m);
```

vector variables only

Lack of Auto-Differentiation

Lack of GPU Support

No native support of tensor variables

⇒ impossible to do deep learning with GRANSO

GRANSO meets PyTorch



NCVX PyGRANSO
Documentation

Search the docs ...

Introduction

Installation

Settings

Examples



NCVX Package

NCVX: A General-Purpose Optimization Solver for Constrained Machine and Deep Learning

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{x}), \text{ s.t. } c_i(\mathbf{x}) \leq 0, \forall i \in \mathcal{I}; c_i(\mathbf{x}) = 0, \forall i \in \mathcal{E}$$

First general-purpose solver for constrained DL problems

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- Why CDL
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- **PyGranso in action**
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Example 1: Support Vector Machine (SVM)

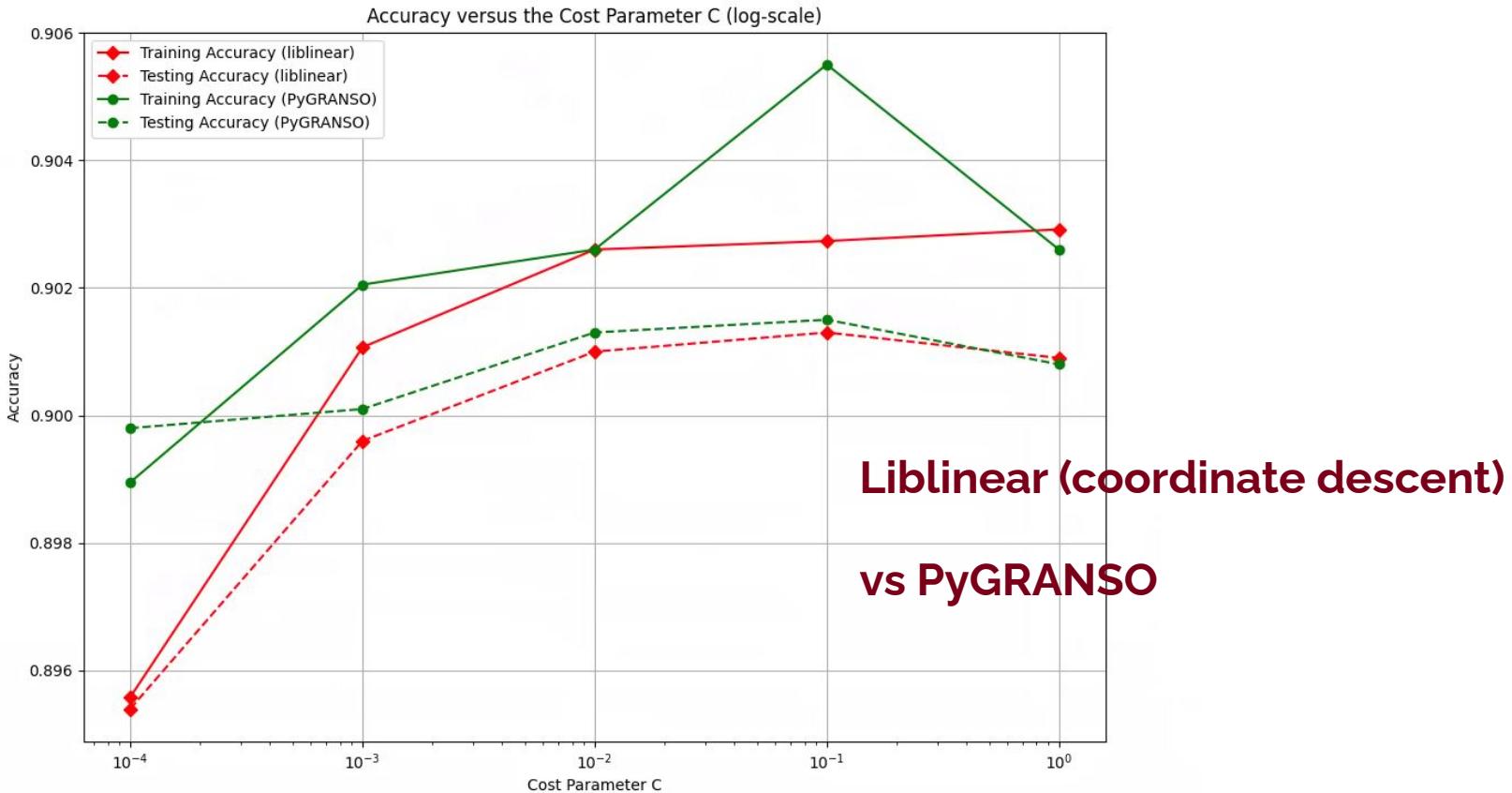
Soft-margin SVM

$$\min_{\mathbf{w}, b, \zeta} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^n \zeta_i$$

$$\text{s.t. } y_i (\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 - \zeta_i, \quad \zeta_i \geq 0 \quad \forall i = 1, \dots, n$$

```
def comb_fn(X_struct):
    # obtain optimization variables
    w = X_struct.w
    b = X_struct.b
    zeta = X_struct.zeta
    # objective function
    f = 0.5*w.T@w + C*torch.sum(zeta)
    # inequality constraints
    ci = pygransoStruct()
    ci.c1 = 1 - zeta - y*(x@w+b)
    ci.c2 = -zeta
    # equality constraint
    ce = None
    return [f,ci,ce]
# specify optimization variables
var_in = {"w": [d,1], "b": [1,1], "zeta": [n,1]}
# pygranso main algorithm
soln = pygranso(var_in,comb_fn)
```

Binary classification (odd vs even digits) on MNIST dataset



Example 2: Robustness—min formulation

$$\min_{\mathbf{x}'} d(\mathbf{x}, \mathbf{x}')$$

$$\text{s. t. } \max_{\ell \neq c} f_{\boldsymbol{\theta}}^{\ell}(\mathbf{x}') \geq f_{\boldsymbol{\theta}}^c(\mathbf{x}')$$

$$\mathbf{x}' \in [0, 1]^n$$

```
def comb_fn(X_struct):
    # obtain optimization variables
    x_prime = X_struct.x_prime
    # objective function
    f = d(x,x_prime)
    # inequality constraints
    ci = pygransoStruct()
    f_theta_all = f_theta(x_prime)
    fy = f_theta_all[:,y] # true class output
    # output except true class
    fi = torch.hstack((f_theta_all[:, :y], f_theta_all[:, y+1:]))
    ci.c1 = fy - torch.max(fi)
    ci.c2 = -x_prime
    ci.c3 = x_prime-1
    # equality constraint
    ce = None
    return [f,ci,ce]
# specify optimization variable (tensor)
var_in = {"x_prime": list(x.shape)}
# pygranso main algorithm
soln = pygranso(var_in,comb_fn)
```

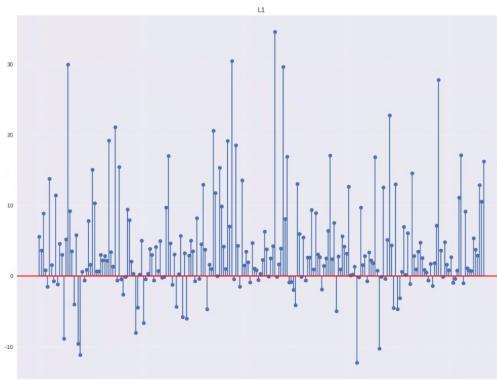
CIFAR10 dataset

Compared with FAB [iterative constraint linearization + projected gradient]

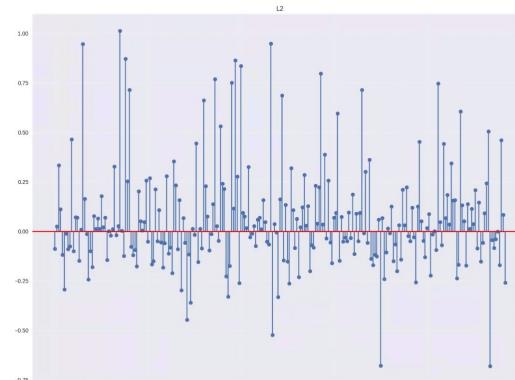
<https://github.com/fra31/auto-attack>

$$\begin{aligned} & \min_{\mathbf{x}'} d(\mathbf{x}, \mathbf{x}') \\ \text{s. t. } & \max_{\ell \neq c} f_{\boldsymbol{\theta}}^{\ell}(\mathbf{x}') \geq f_{\boldsymbol{\theta}}^c(\mathbf{x}') \\ & \mathbf{x}' \in [0, 1]^n \end{aligned}$$

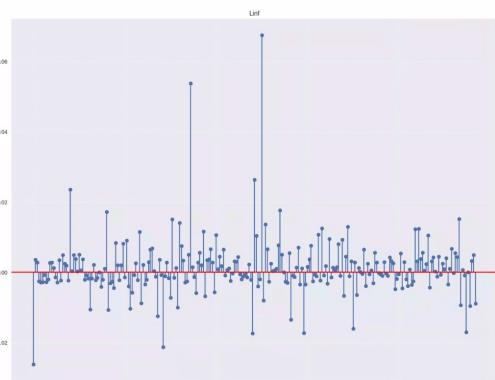
X-axis: image index; Y-axis: PyGRANSO radius - FAB radius



L1 attack



L2 attack



Linf attack

Many
others

<https://ncvx.org/>

NCVX PyGRANSO Documentation

← ⌂ ⌂ ⌂

Search the docs ...

Introduction

Installation

Settings

Examples

Rosenbrock

Eigenvalue Optimization

Dictionary Learning

Nonlinear Feasibility Problem

Sphere Manifold

Trace Optimization

Robust PCA

Generalized LASSO

Logistic Regression

LeNet5

Perceptual Attack

Orthogonal RNN

Highlights

Home



NCVX Package

NCVX (**N**on**C**onVe**X**) is a user-friendly and scalable python software package targeting general nonsmooth NCVX problems with nonsmooth constraints. **NCVX** is being developed by **GLOVEX** at the Department of Computer Science & Engineering, University of Minnesota, Twin Cities.

The initial release of **NCVX** contains the solver **PyGRANSO**, a PyTorch-enabled port of **GRANSO** incorporating auto-differentiation, GPU acceleration, tensor input, and support for new QP solvers. As a highlight, **PyGRANSO** can solve general constrained deep learning problems, the first of its kind.



Closing



Deep Learning with Nontrivial Constraints: Methods and Applications

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NCVX PyGRANSO
Documentation

Search the docs ...

Introduction
Installation
Settings
Examples

Home



NCVX Package

**NCVX: A General-Purpose Optimization Solver for
Constrained Machine and Deep Learning**

Byun Liang, Tim Mitchell, Ju Sun

$$\min_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{x}), \text{ s.t. } c_i(\mathbf{x}) \leq 0, \forall i \in \mathcal{I}; c_i(\mathbf{x}) = 0, \forall i \in \mathcal{E}$$

**First general-purpose solver for constrained DL
problems**

Thanks to all contributors



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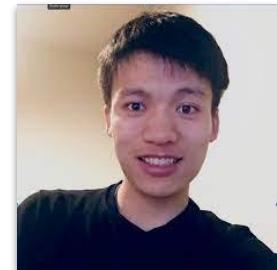
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