Differentiable programming and detector design optimization

Seminaire LPNHE - 14/02/2022

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Outline

Differentiable programming for HEP applications

- (a bit formal) introduction to **automatic differentiation**
- **Optimization** use-cases: **analysis** optimization, detector **design**
- **MODE** collaboration
- Ongoing **projects**

Acknowledgements

Many of the material presented in this talk was shown at the **1st Workshop on Differentiable Programming** for experimental design organised by the **MODE collaboration** last September

Thanks to

Atilim Gunes Baydin

Tommaso Dorigo

Giles Strong

Nathan Simpson

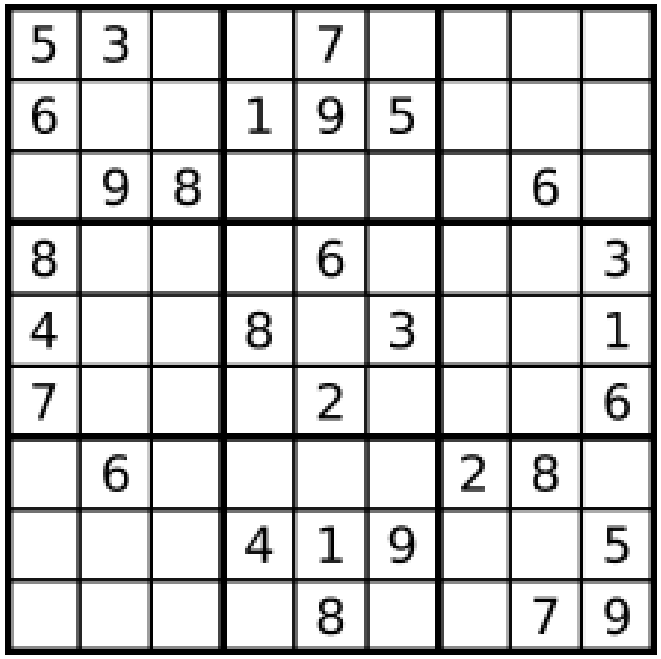
...

https://indico.cern.ch/event/1022938/

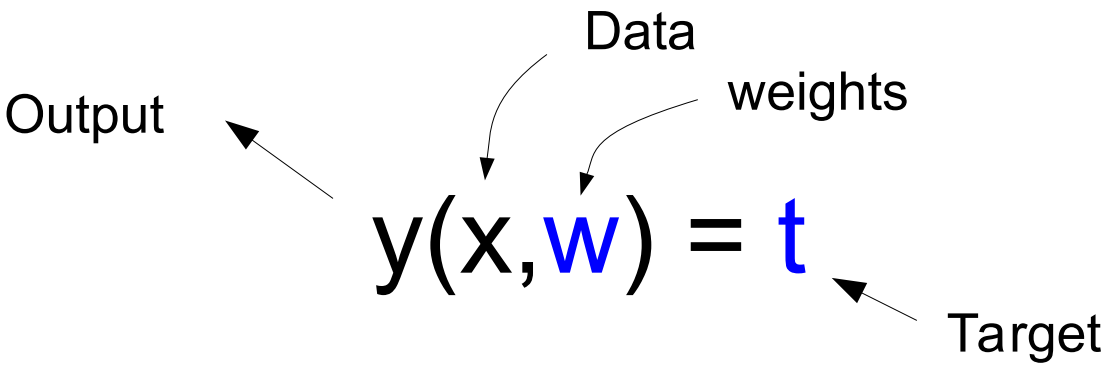
Disclaimer

“You know nothing, Jon Snow”

Warm up: ML basics

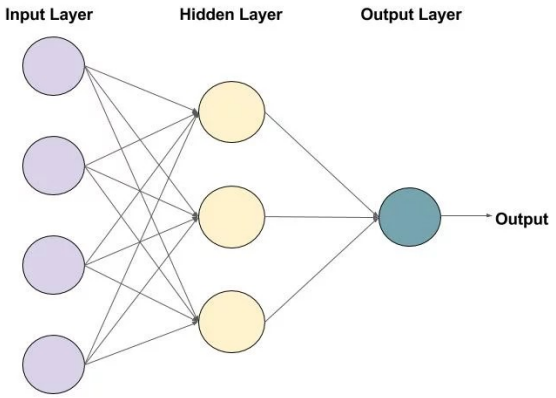


Machine Learning Basics



Training Neural Networks

Data
(features **x**)



Objective
(target **t**)

y = f(**x**, **W**)

f : non-linear functions
W : parameters (weights)

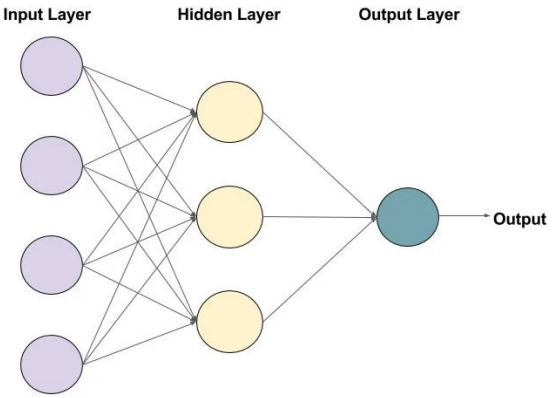
Cost function

"how close is the network output to the objective ?"

$\ell(\mathbf{y}, \mathbf{t})$

Training Neural Networks

Data
(features **x**)



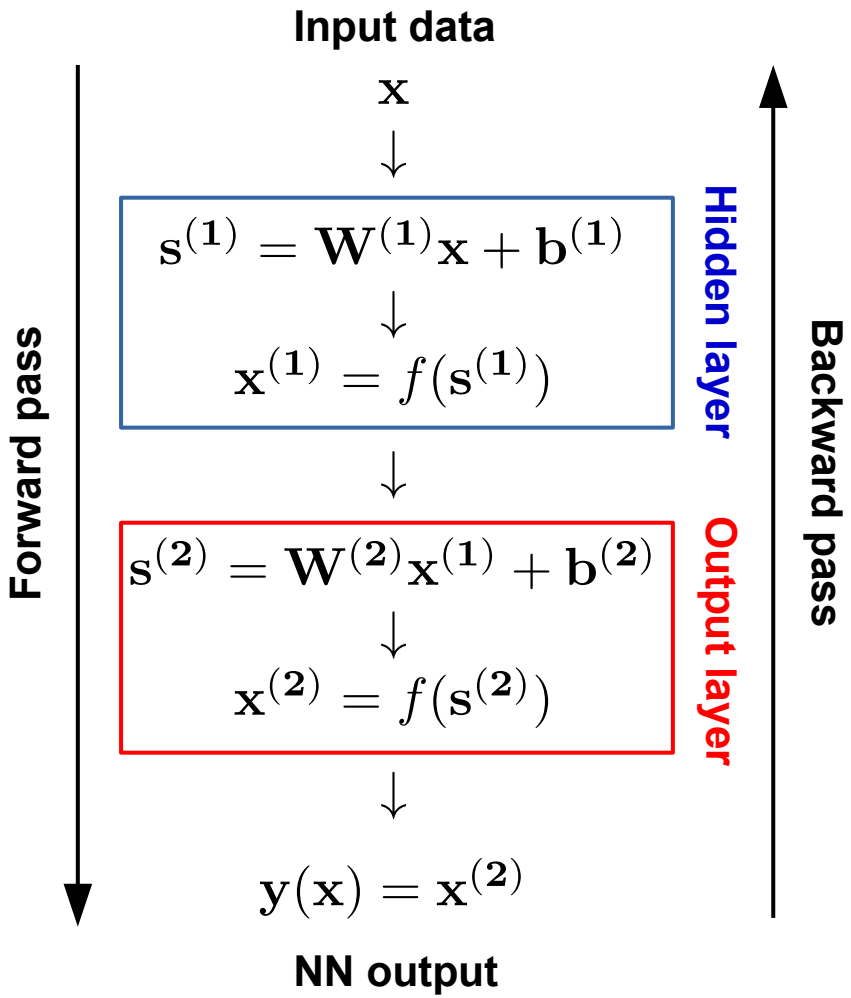
Objective
(target **t**)

Update of weights **W**

$$\mathbf{W} \rightarrow \mathbf{W} - \eta \sum_{N} \frac{\partial \ell(\mathbf{y}, \mathbf{t})}{\partial \mathbf{W}}$$

Backpropagation in NN

Example: MLP network with 2 layers (1 hidden, 1 output)

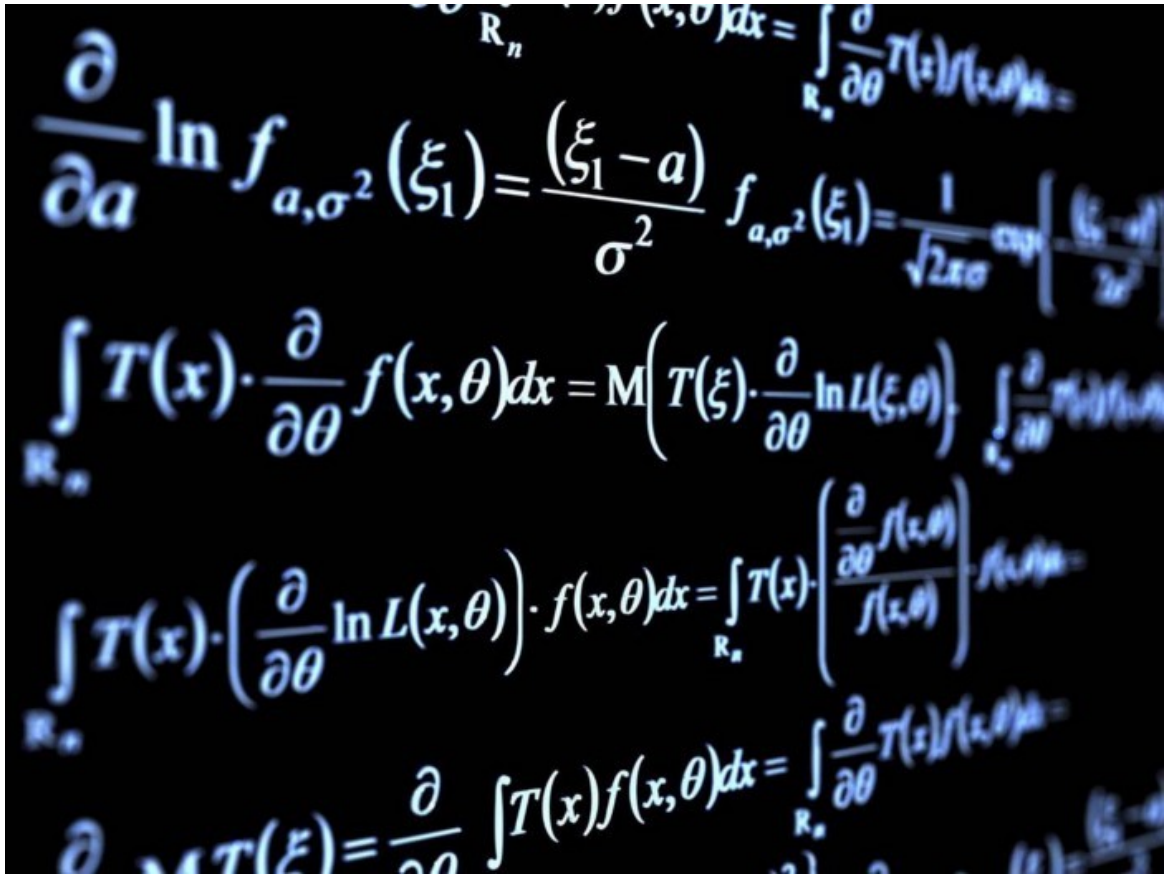


Use chain rule to compute derivatives of the loss $\ell(\mathbf{y}, \mathbf{t})$

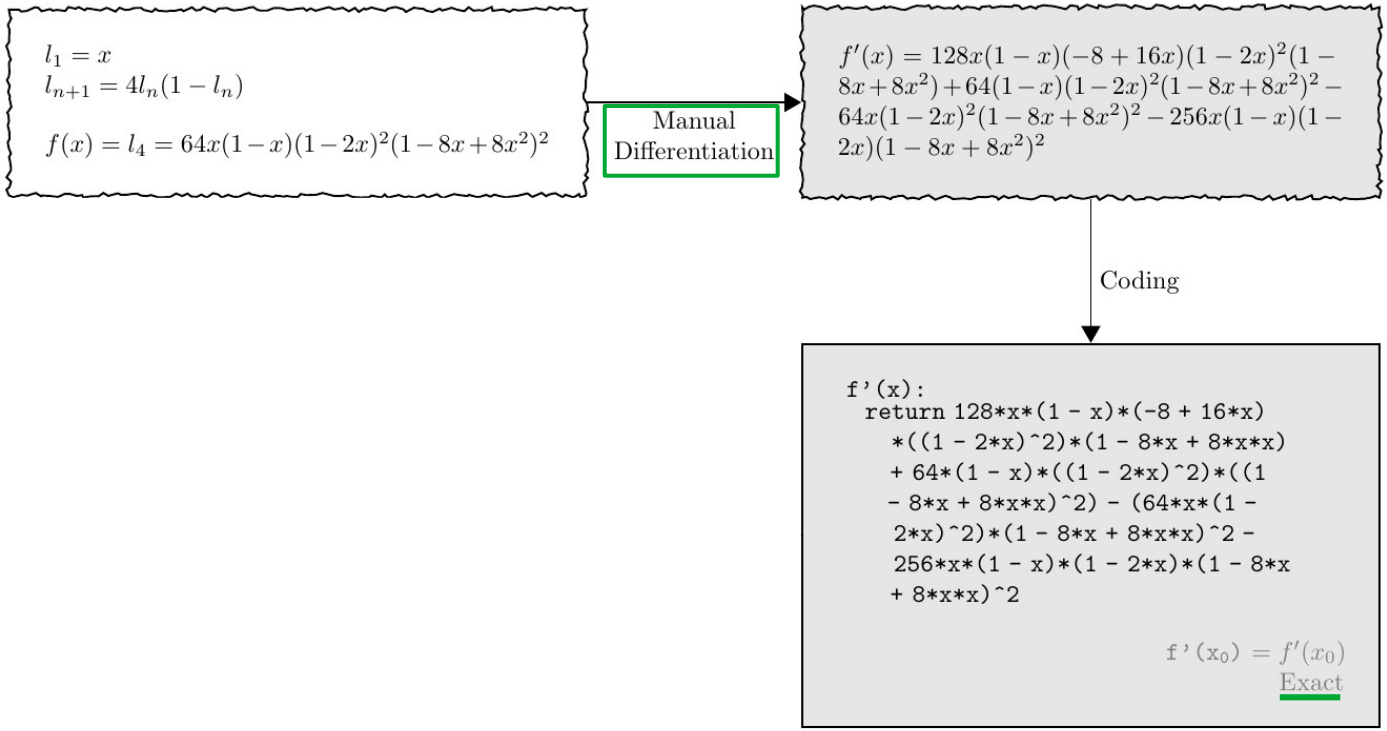
$$\frac{\partial \ell}{\partial \mathbf{W}^{(2)}} = \frac{\partial \ell}{\partial \mathbf{y}} \frac{\partial \mathbf{y}}{\partial \mathbf{s}^{(2)}} \frac{\partial \mathbf{s}^{(2)}}{\partial \mathbf{W}^{(2)}}$$
$$= \frac{\partial \ell}{\partial \mathbf{y}} \frac{\partial f(\mathbf{s}^{(2)})}{\partial \mathbf{s}^{(2)}} \mathbf{x}^{(1)}$$

$$\frac{\partial \ell}{\partial \mathbf{W}^{(1)}} = \frac{\partial \ell}{\partial \mathbf{y}} \frac{\partial \mathbf{y}}{\partial \mathbf{s}^{(2)}} \frac{\partial \mathbf{s}^{(2)}}{\partial \mathbf{x}^{(1)}} \frac{\partial \mathbf{x}^{(1)}}{\partial \mathbf{s}^{(1)}} \frac{\partial \mathbf{s}^{(1)}}{\partial \mathbf{W}^{(1)}}$$
$$= \frac{\partial \ell}{\partial \mathbf{y}} \frac{\partial f(\mathbf{s}^{(2)})}{\partial \mathbf{s}^{(2)}} \frac{\partial \mathbf{s}^{(2)}}{\partial \mathbf{x}^{(1)}} \frac{\partial f(\mathbf{s}^{(1)})}{\partial \mathbf{s}^{(1)}} \mathbf{x}$$

Automatic differentiation



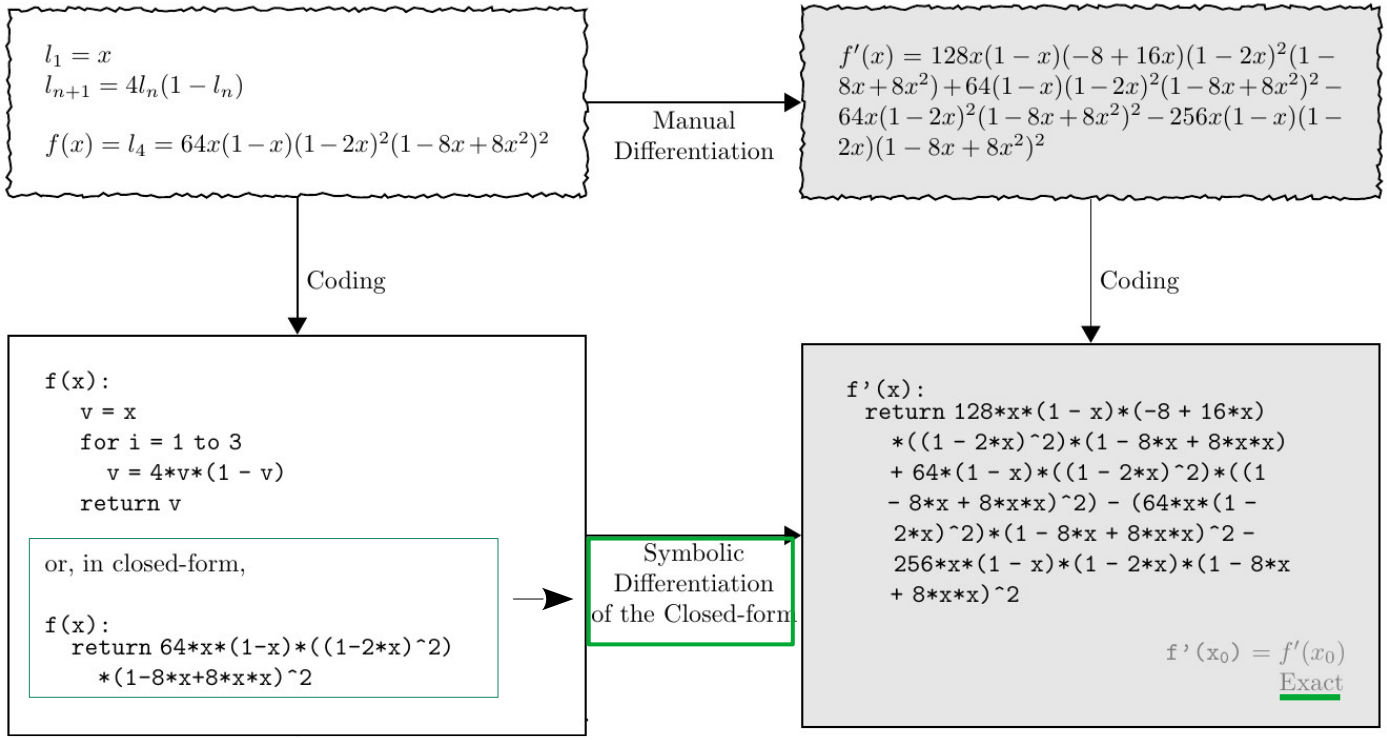
How to code derivatives ?



(Note: numerical differentiation is also an option but it gives approximate results)

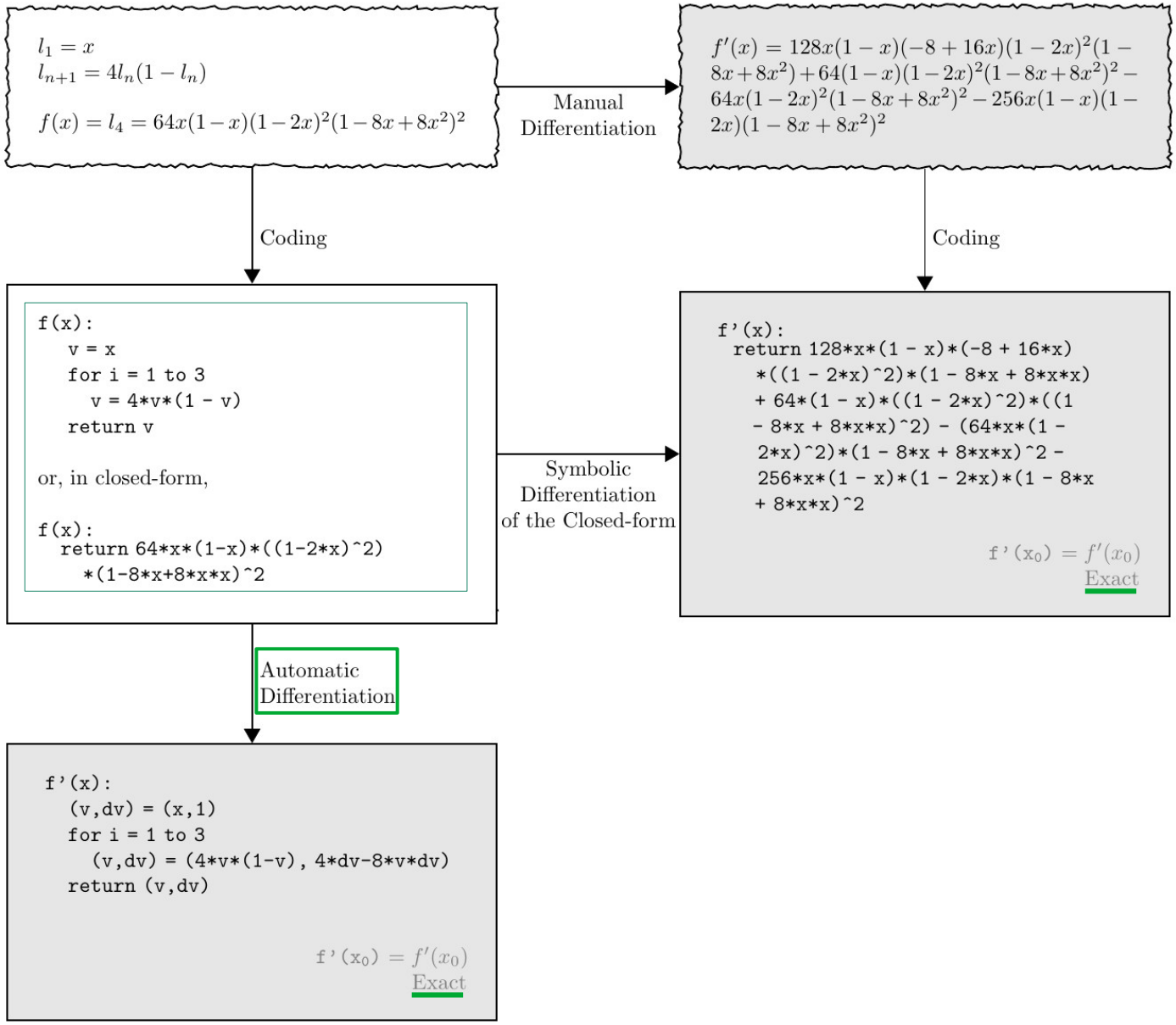
Baydin et al.
[1502.05767]

How to code derivatives ?



Baydin et al.
[1502.05767]

How to code derivatives ?



Baydin et al.
[1502.05767]

Automatic differentiation

Automatic (algorithmic) differentiation (AD)

- **Numerical derivative evaluations** rather than derivative **expressions**
- Composition of **operations** for which **derivatives are known**
- **No need to rearrange** the code in a closed-form expression
- Accurate at **machine precision**

For each function a **computational graph** is constructed
→ **evaluation** of the function (forward pass)
→ calculation of **gradient** (backward pass)

Computational graph (example)

Forward pass

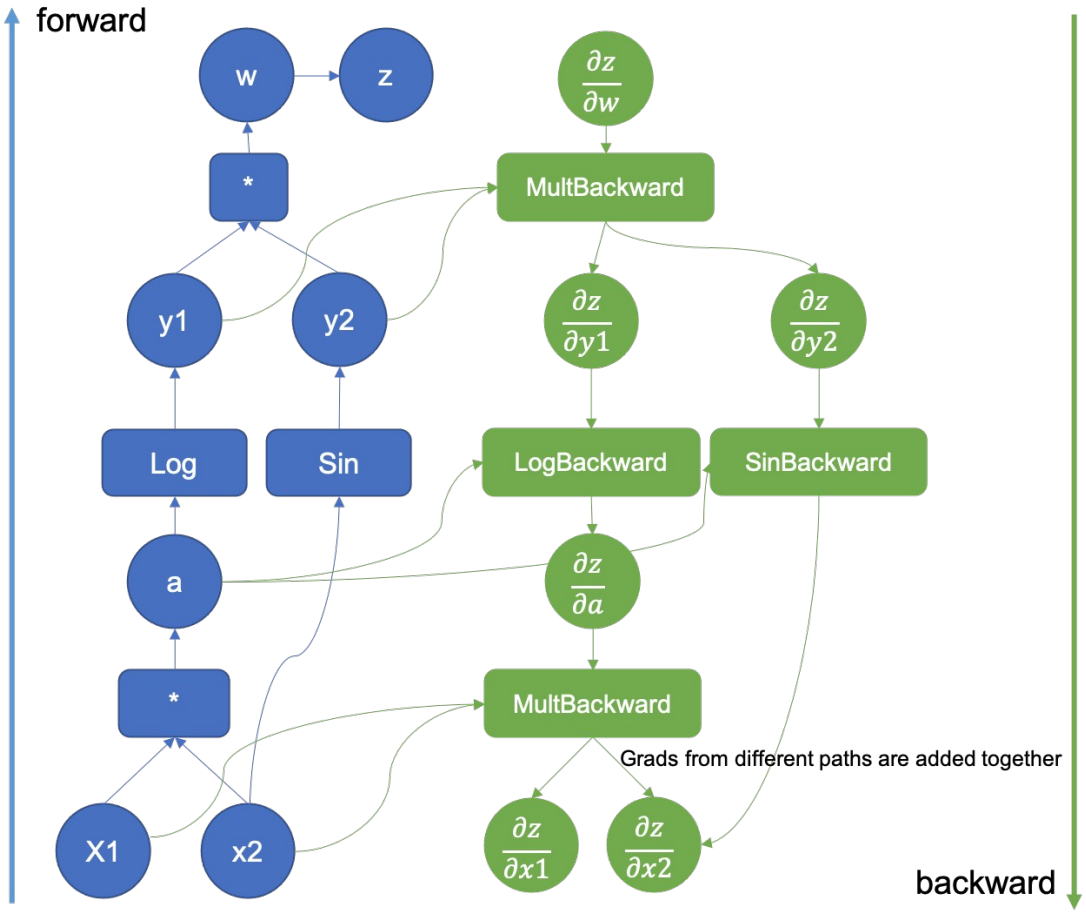
$$\vec{y} = \begin{pmatrix} \log(x_1 x_2) \\ \sin(x_2) \end{pmatrix}$$

$$z = y_1 y_2$$

Backward pass

$$\begin{pmatrix} \frac{\partial z}{\partial x_1} \\ \frac{\partial z}{\partial x_2} \end{pmatrix} = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} \end{pmatrix}^T \begin{pmatrix} \frac{\partial z}{\partial y_1} \\ \frac{\partial z}{\partial y_2} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{y_2}{x_1} \\ \frac{y_2}{x_2} + y_1 \cos(x_1) \end{pmatrix}$$

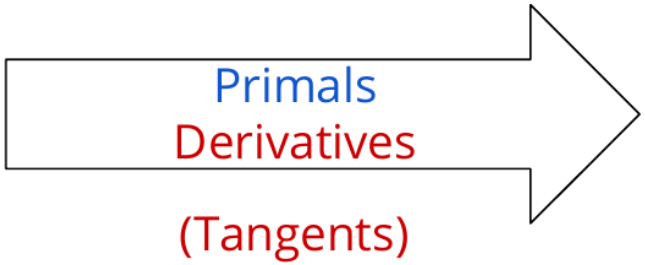


(see: https://pytorch.org/blog/overview-of-pytorch-autograd-engine/)

Automatic differentiation

Two **main modes**, both based on chain rule

Forward mode

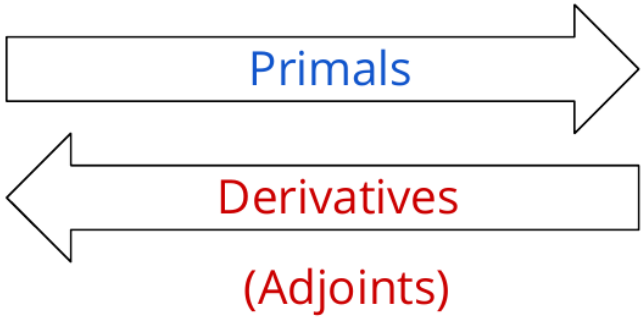


Associate each **intermediate variable** v_i with a derivative $\dot{v}_i = \frac{\partial v_i}{\partial x}$

Apply chain rule to each **elementary operations** in Forward propagation

Best suited for $f : \mathbb{R}^n \to \mathbb{R}^m, n \ll m$

Reverse mode (backpropagation)



Propagates derivatives **backwards from output** $\bar{v}_i = \frac{\partial f}{\partial v_i}$

Two phases

1. Calculate **intermediate** variables v_i
2. Calculate **derivatives**: output → input

Best suited for $f : \mathbb{R}^n \to \mathbb{R}^m, m \ll n$

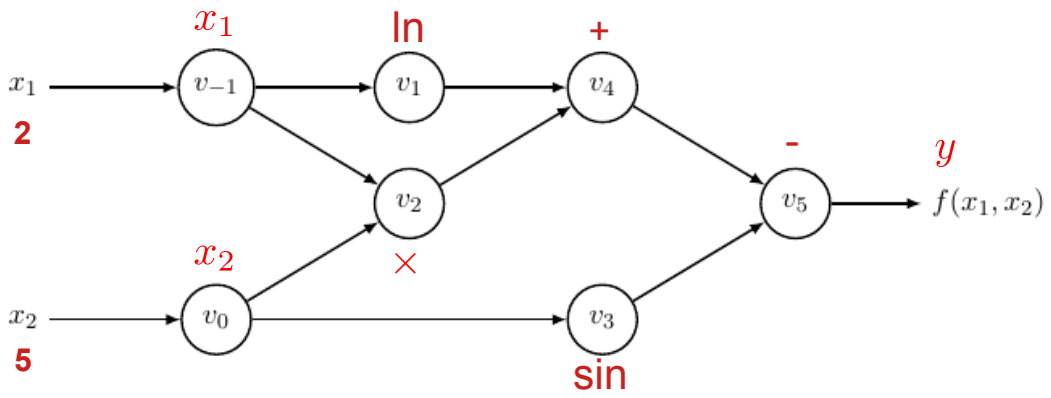
[figure G. Baydin]

Forward mode

Example

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)$$

Each **intermediate variable** is associated to $\dot{v}_i = \frac{\partial v_i}{\partial x}$



Forward Primal Trace			Forward Tangent (Derivative) Trace		
v_{-1}	$= x_1$	$= 2$	$\dot{v}_{-1}$	$= \dot{x}_1$	$= 1$
v_0	$= x_2$	$= 5$	$\dot{v}_0$	$= \dot{x}_2$	$= 0$
v_1	$= \ln v_{-1}$	$= \ln 2$	$\dot{v}_1$	$= \dot{v}_{-1}/v_{-1}$	$= 1/2$
v_2	$= v_{-1} \times v_0$	$= 2 \times 5$	$\dot{v}_2$	$= \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1}$	$= 1 \times 5 + 0 \times 2$
v_3	$= \sin v_0$	$= \sin 5$	$\dot{v}_3$	$= \dot{v}_0 \times \cos v_0$	$= 0 \times \cos 5$
v_4	$= v_1 + v_2$	$= 0.693 + 10$	$\dot{v}_4$	$= \dot{v}_1 + \dot{v}_2$	$= 0.5 + 5$
v_5	$= v_4 - v_3$	$= 10.693 + 0.959$	$\dot{v}_5$	$= \dot{v}_4 - \dot{v}_3$	$= 5.5 - 0$
y	$= v_5$	$= 11.652$	$\dot{y}$	$= \dot{v}_5$	$= 5.5$

$\dot{v}_i = \frac{\partial v_i}{\partial x_1}$

Forward mode example, evaluated at (x_1, x_2) = (2, 5) and setting $\dot{x}_1 = 1$ to compute $\dot{y} = \frac{\partial y}{\partial x_1}$

[1502.05767]

Digression: Dual numbers

Forward mode can be viewed as evaluating a function using **dual numbers**

Numbers defined as $v + \dot{v}\epsilon$ where $\epsilon \neq 0$ and $\epsilon^2 = 0$

Properties (using Taylor expansion):

$$f(v + \dot{v}\epsilon) = f(v) + f'(v)\dot{v}\epsilon$$

$$\begin{aligned} f(g(v + \dot{v}\epsilon)) &= f(g(v) + g'(v)\dot{v}\epsilon)) \\ &= f(g(v)) + f'(g(v))g'(v)\dot{v}\epsilon \end{aligned}$$

Composite function derivative !

In practice, implement **specific code** to handle the **dual operations** so that **function f and its derivative are simultaneously computed** (operator overloading)

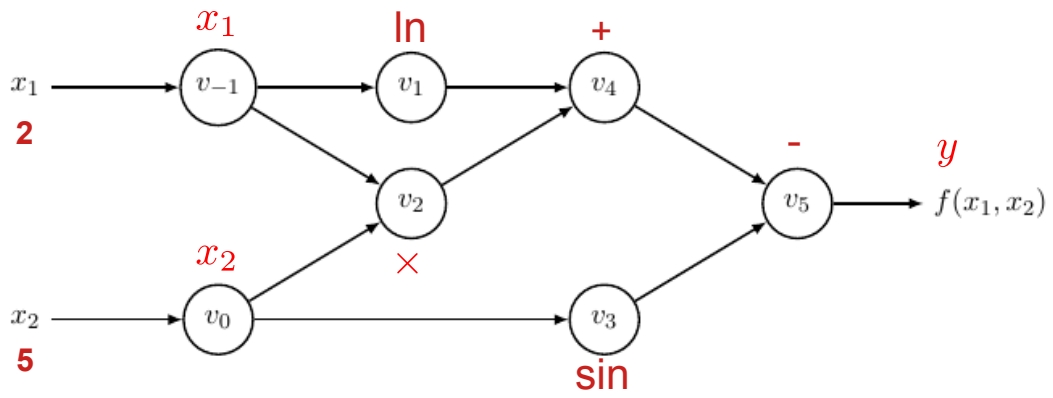
(For a concrete example with code see R. Lange post)

Reverse mode (backpropagation)

Example

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)$$

Propagates derivatives **backwards** from output $\bar{v}_i = \dfrac{\partial y}{\partial v_i}$



Forward Primal Trace		
$v_{-1} = x_1$	$= 2$	
$v_0 = x_2$	$= 5$	
$v_1 = \ln v_{-1}$	$= \ln 2$	
$v_2 = v_{-1} \times v_0$	$= 2 \times 5$	
$v_3 = \sin v_0$	$= \sin 5$	
$v_4 = v_1 + v_2$	$= 0.693 + 10$	
$v_5 = v_4 - v_3$	$= 10.693 + 0.959$	
$y = v_5$	$= 11.652$	

Reverse Adjoint (Derivative) Trace		
$\bar{x}_1 = \bar{v}_{-1}$		$= \mathbf{5.5}$
$\bar{x}_2 = \bar{v}_0$		$= \mathbf{1.716}$
$\bar{v}_{-1} = \bar{v}_{-1} + \bar{v}_1 \frac{\partial v_1}{\partial v_{-1}}$	$= \bar{v}_{-1} + \bar{v}_1 / v_{-1}$	$= 5.5$
$\bar{v}_0 = \bar{v}_0 + \bar{v}_2 \frac{\partial v_2}{\partial v_0}$	$= \bar{v}_0 + \bar{v}_2 \times v_{-1}$	$= 1.716$
$\bar{v}_{-1} = \bar{v}_2 \frac{\partial v_2}{\partial v_{-1}}$	$= \bar{v}_2 \times v_0$	$= 5$
$\bar{v}_0 = \bar{v}_3 \frac{\partial v_3}{\partial v_0}$	$= \bar{v}_3 \times \cos v_0$	$= -0.284$
$\bar{v}_2 = \bar{v}_4 \frac{\partial v_4}{\partial v_2}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_1 = \bar{v}_4 \frac{\partial v_4}{\partial v_1}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3}$	$= \bar{v}_5 \times (-1)$	$= -1$
$\bar{v}_4 = \bar{v}_5 \frac{\partial v_5}{\partial v_4}$	$= \bar{v}_5 \times 1$	$= 1$
$\bar{v}_5 = \bar{y}$	$= 1$	

Reverse mode example, evaluated at (x_1, x_2) = (2, 5). Both $\dfrac{\partial y}{\partial x_1}$ and $\dfrac{\partial y}{\partial x_2}$ are computed on the same reverse pass starting from the output

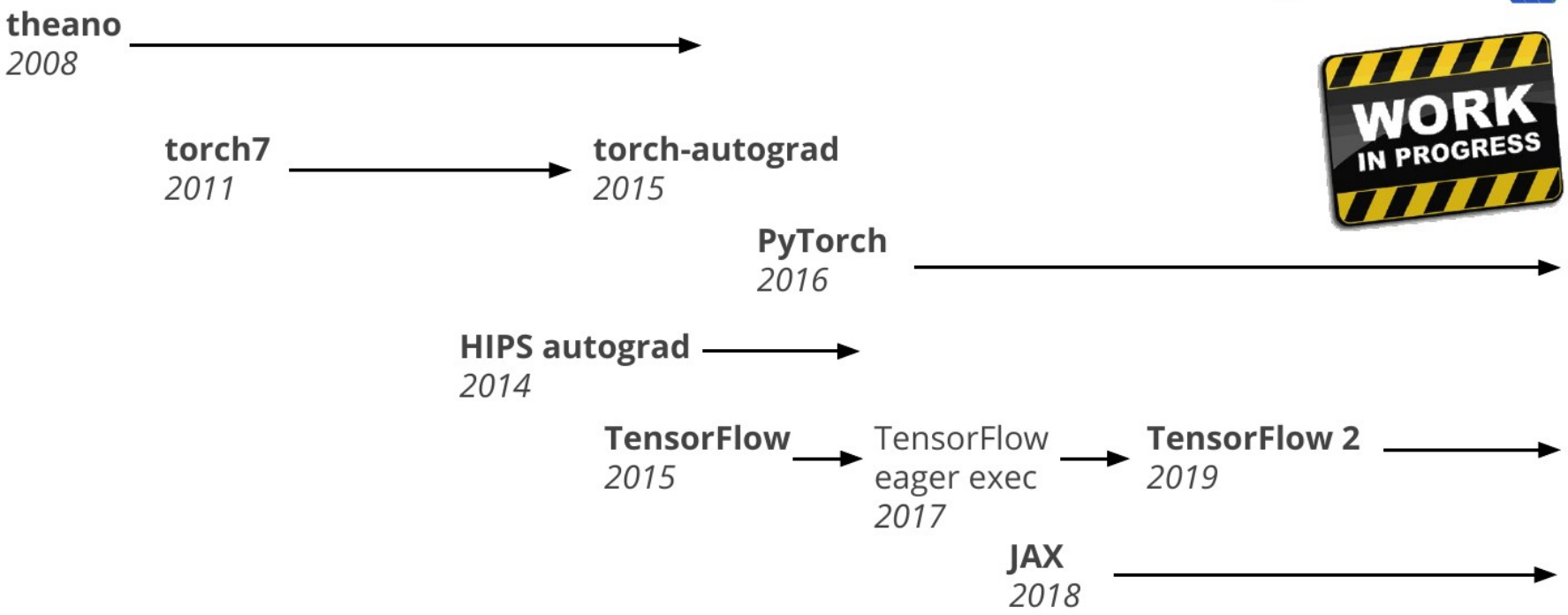
$$\bar{v}_5 = \bar{y} = \frac{\partial y}{\partial y} = 1$$

[1502.05767]

Current state of differentiable programming

Evolution of frameworks

From: **coarse-grained (module level) backprop**
Towards: **fine-grained, general-purpose automatic differentiation**



Auto-diff tools: http://www.autodiff.org/

[slide G. Baydin]

Pytorch example (simple)

PyTorch enables automatic **differentiation** of **computational graphs**

Example: differentiation of $f(x) = x^4$

Pure python

```
f = 1
for i in range(4):
    f = f * x
```


```
def fun(x):
    return x.pow(4)

x = torch.tensor(2.,requires_grad=True)
f = fun(x)
```

```
f.backward()
```

← $\frac{\mathrm{d}f}{\mathrm{d}x}(x)$

```
torch.autograd.functional.hessian(fun,x)
```

← $\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}(x)$

→ f(2) = 16, f'(2) = 32, f''(2) = 48

Note: exact numerical value of derivative is computed (no analytical form)

Pytorch example (differential geometry)

Calculate **partial derivatives** of metric tensor w.r.t to coordinates $x^\alpha = (ct, r, \theta, \phi)$

$$g_{\mu\nu} = \begin{pmatrix} 1 - \frac{R_s}{R} & 0 & 0 & 0 \\ 0 & -\left(1 - \frac{R_s}{R}\right)^{-1} & 0 & 0 \\ 0 & 0 & -R^2 & 0 \\ 0 & 0 & 0 & -R^2 \sin^2\theta \end{pmatrix}$$

Jacobian matrix:

```
grad = functional.jacobian(metric_tensor,coord)
print(grad.T)
```

→ $\frac{\partial g_{\mu\nu}}{\partial x^\alpha}$ (4 matrices)

2nd order derivatives:

```
def fgrad(inputs):
    return torch.autograd.functional.jacobian(metric_tensor,inputs, create_graph=True)

hessian = torch.autograd.functional.jacobian(fgrad,coord, create_graph=True)
print(hessian)
```

→ $\frac{\partial^2 g_{\mu\nu}}{\partial x^\alpha \partial x^\beta}$ (16 matrices)

Differentiable programming

Gradient-based **optimization** methods:

- ➔ Code composed of **differentiable and parameterized building blocks**
- ➔ **Software** optimized via **automatic differentiation**

Differentiable programming in HEP

Incorporating automatic differentiation in HEP software

In Analysis Code

- **Optimize** free **parameters** with respect to the **desired physics objective**
- End-to-end **differentiable** analysis **workflow**

In Simulation Code

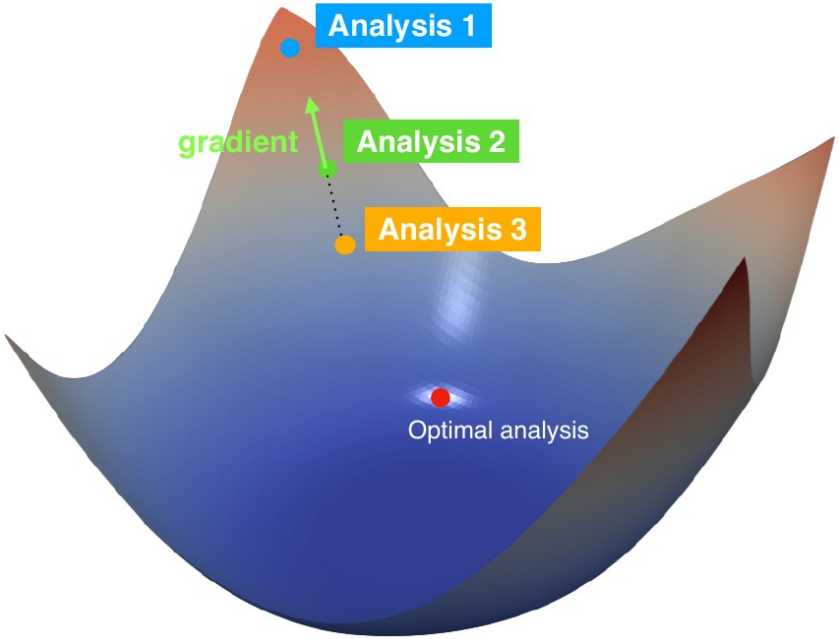
- Compute gradient for with respect to **parameters of simulation**
- EFT, Cosmology, MadGraph (evaluation of matrix element), …

Differentiable programming in High Energy Physics, SnowMass 2021

Differentiable analysis: NEOS

End-to-end optimized **analysis pipelines** that use the **analysis sensitivity** including **systematic** uncertainties as the **objective** function

github.com/gradhep/neos



[figure N. Simpson]

Differentiable analysis: NEOS

End-to-end optimized **analysis pipelines** that use the **analysis sensitivity** including **systematic** uncertainties as the **objective** function

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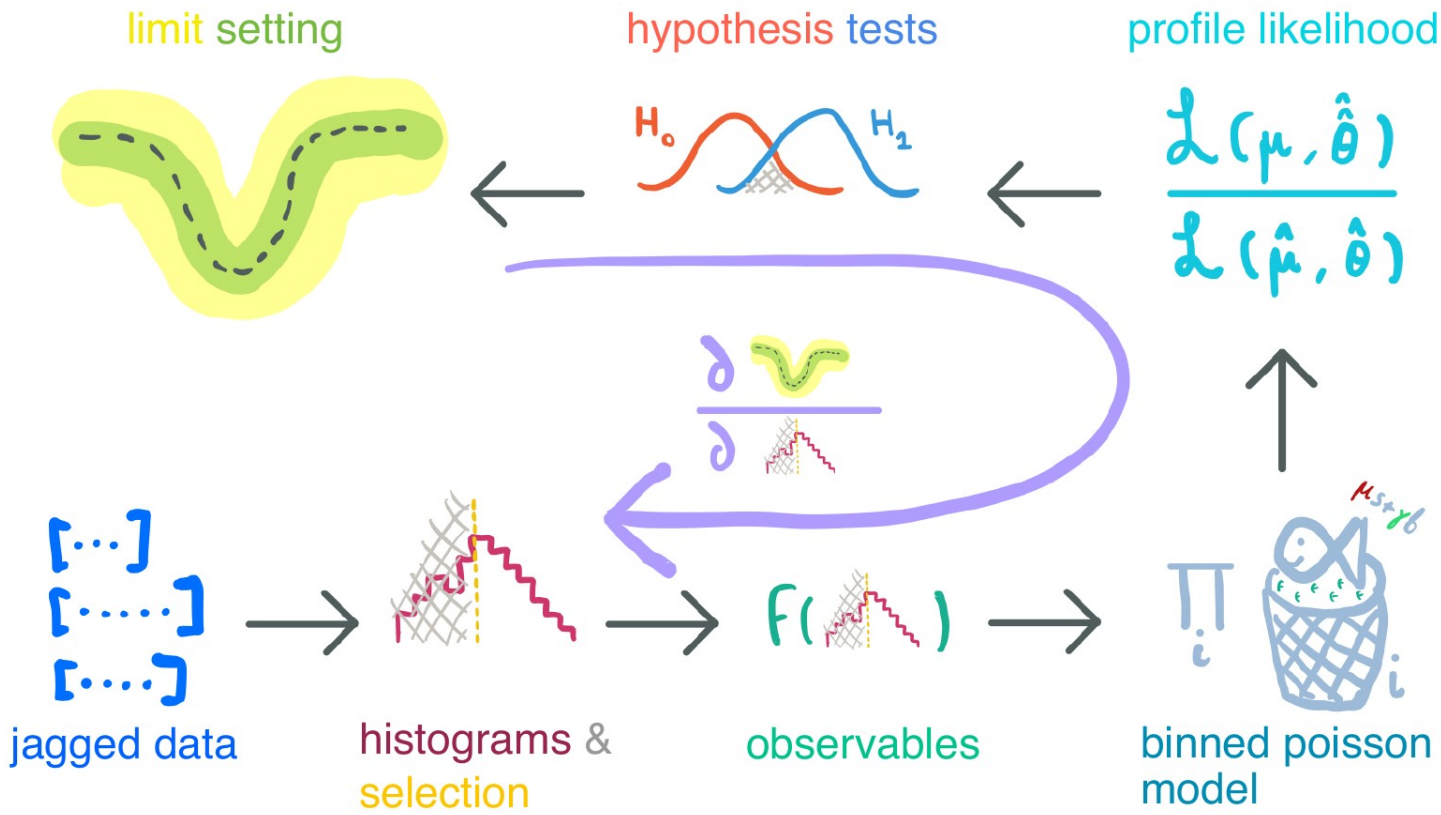
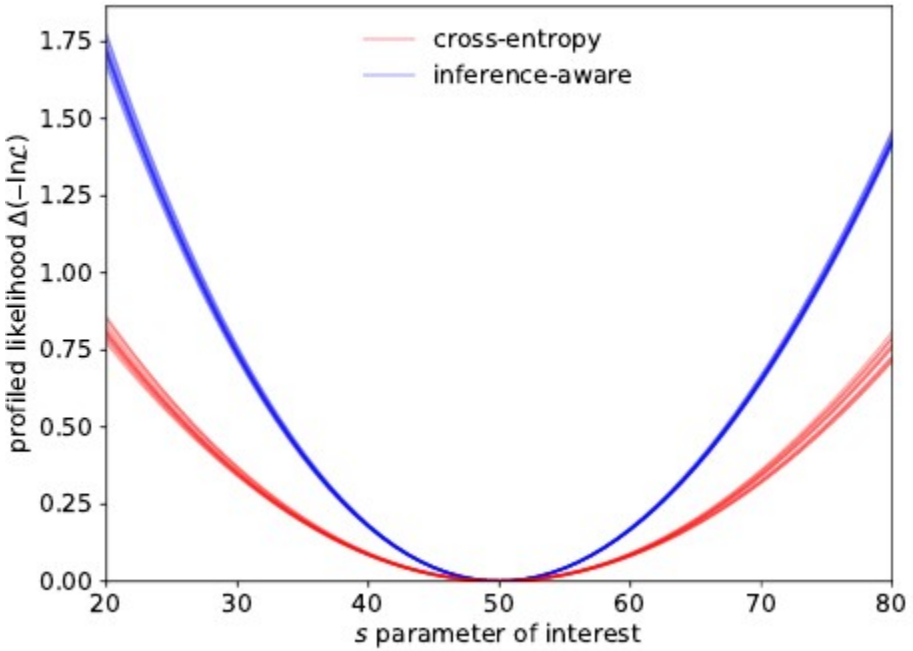


[Slide Nathan Simpson]

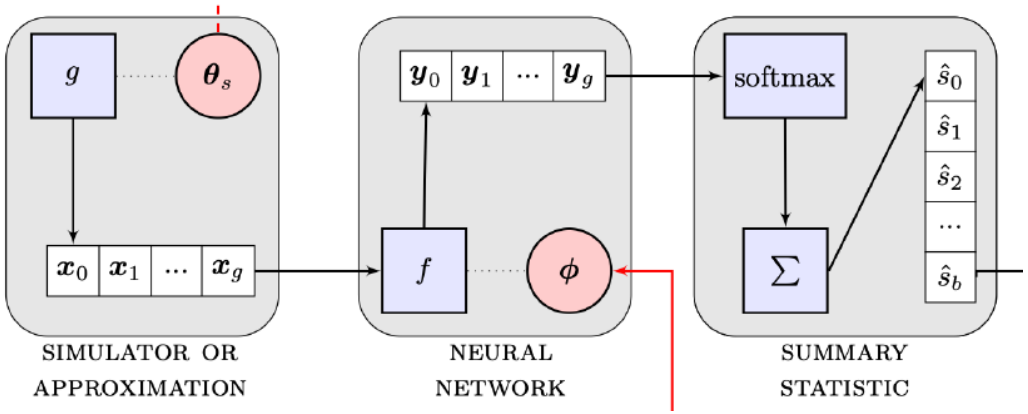
Inference Aware **N**eural **O**ptimization [1806.04743, de Castro, Dorigo]

- **Include nuisance parameters** in the loss function and directly minimize **precision of parameters of interest** (e.g. signal strenght measurement)

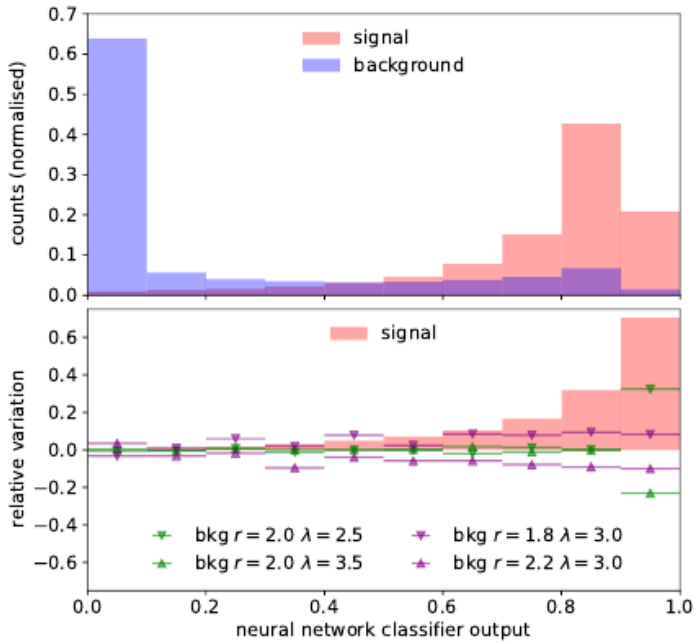


Profiled likelihood around the expectation value for the parameter of interest for **inference-aware** models and **cross-entropy** loss based models.

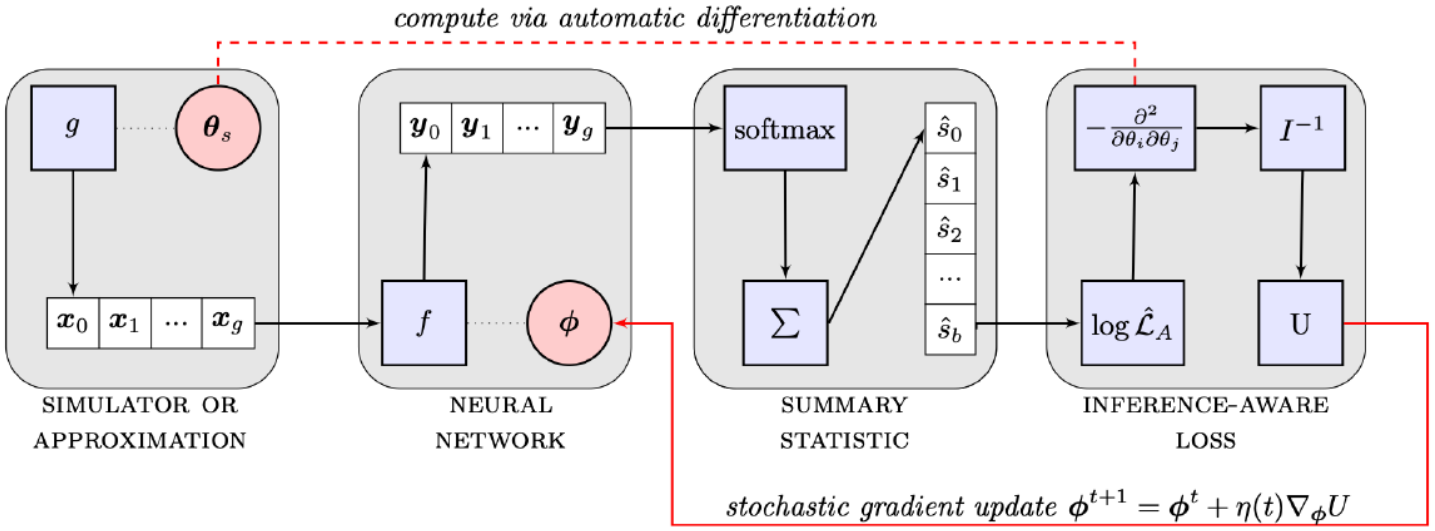
INFERNO algorithm



NN output →



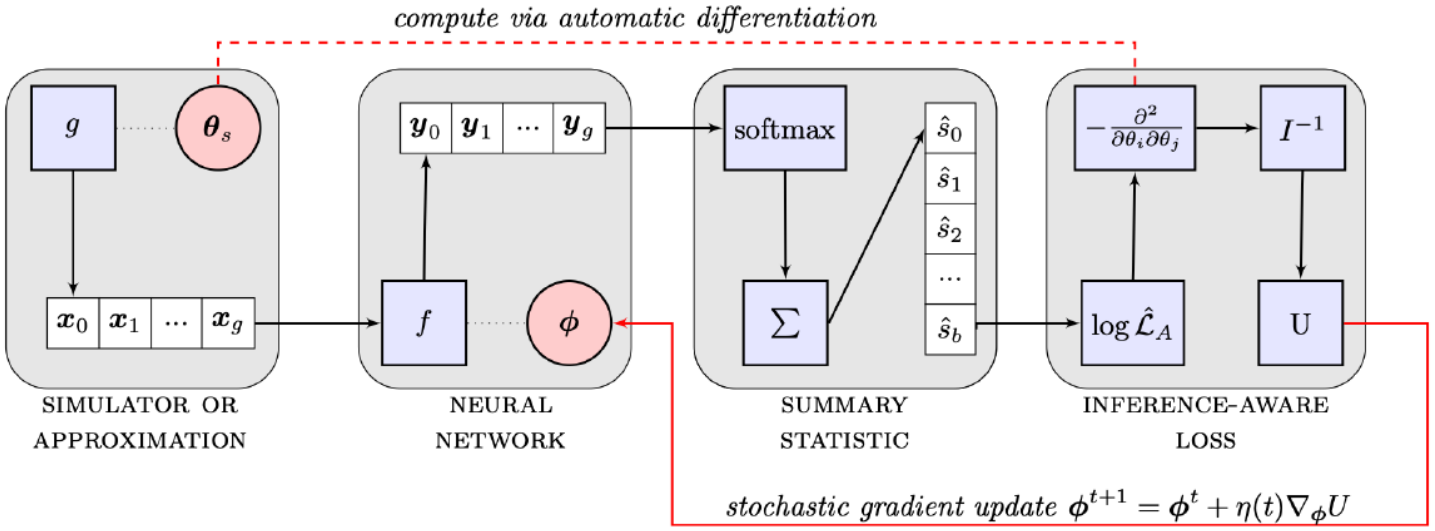
INFERNO algorithm



NN **loss** function: **uncertainty** on parameter of interest (U)

Obtained by computing full **hessian** of the **Likelihood** with respect to all **nuisance** parameters

INFERNO algorithm



Algorithm 1 Inference-Aware Neural Optimisation.

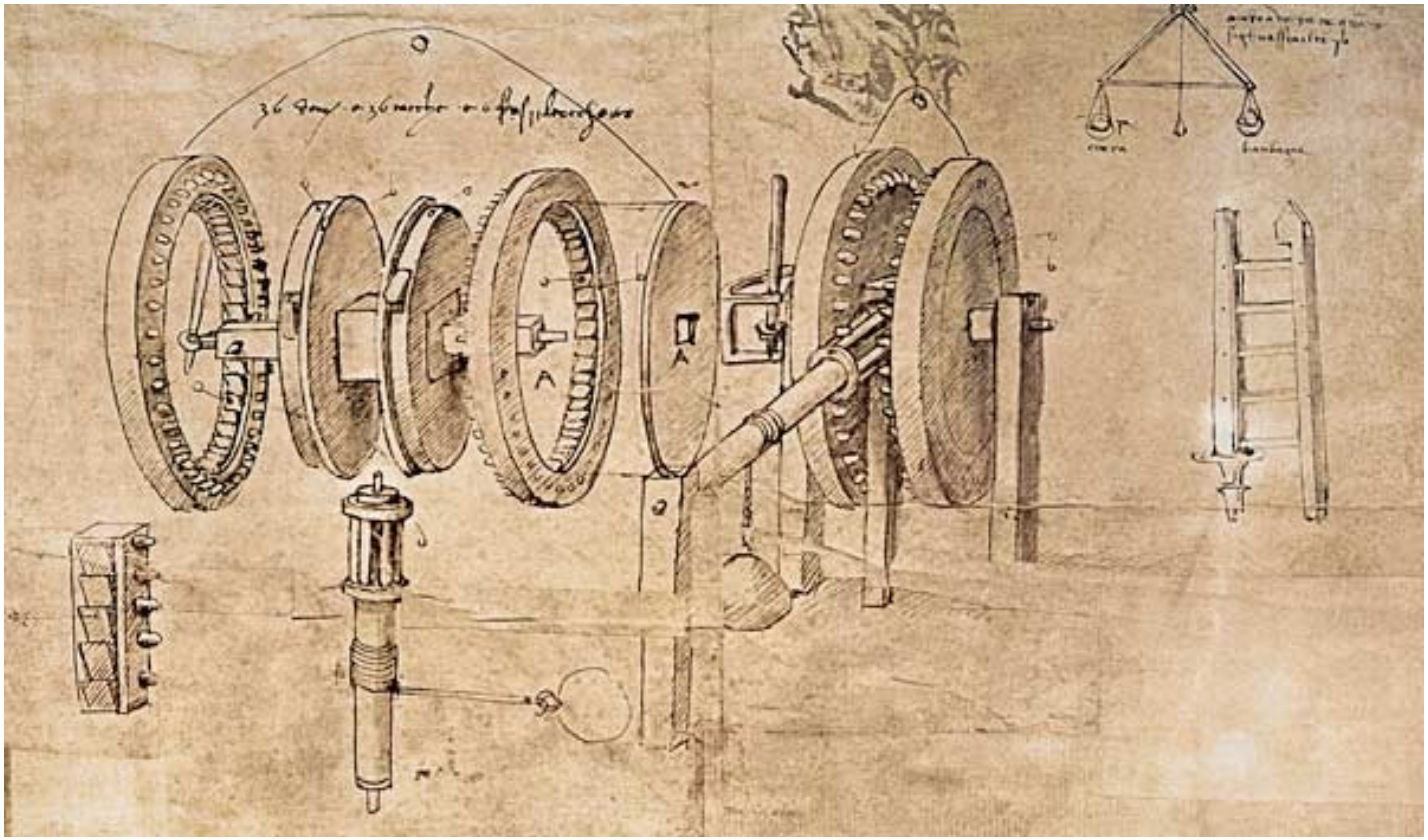
Input 1: differentiable simulator or variational approximation $g(\boldsymbol{\theta})$.
Input 2: initial parameter values $\boldsymbol{\theta}_s$.
Input 3: parameter of interest $\omega_0 = \theta_k$.
Output: learned summary statistic $\boldsymbol{s}(D;\boldsymbol{\phi})$.

1: **for** $i = 1$ to N **do**
2: Sample a representative mini-batch G_s from $g(\boldsymbol{\theta}_s)$.
3: Compute differentiable summary statistic $\hat{\boldsymbol{s}}(G_s;\boldsymbol{\phi})$.
4: Construct Asimov likelihood $\mathcal{L}_A(\boldsymbol{\theta},\boldsymbol{\phi})$.
5: Get information matrix inverse $I(\boldsymbol{\theta})^{-1} = \boldsymbol{H}_{\boldsymbol{\theta}}^{-1}(\log\mathcal{L}_A(\boldsymbol{\theta},\boldsymbol{\phi}))$.
6: Obtain loss $U = I_{kk}^{-1}(\boldsymbol{\theta}_s)$.
7: Update network parameters $\boldsymbol{\phi} \rightarrow \text{SGD}(\nabla_{\boldsymbol{\phi}}U)$.
8: **end for**

For a detailed explanation of the algorithm see G. Strong blog post

Optimization of detector design

Can automatic differentiation be applied to detector optimization ?



Optimization of detector design

Design of detectors traditionally **relies** on individual **optimization of subdetector**

- **Track first, destroy later**
  - First detect ionization tracks in tracker, then measure energy deposits from destructive interaction with thick calorimeters
- **Per-subdetector optimization**
  - subdetector-specific figures of merit (e.g. momentum resolution)
- **Impact on physics goals** typically considered in a second step

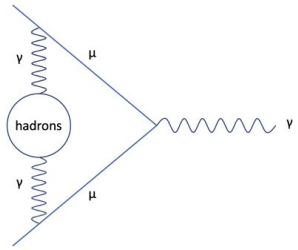
Optimization of a **joint problem** ≠ different from **individual optimization**

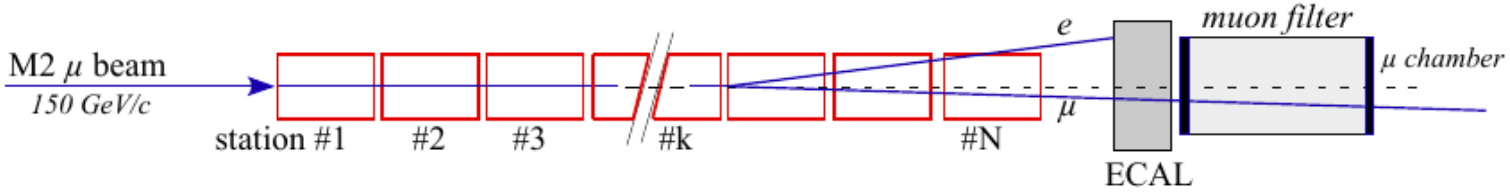
$$argmax_{x,y}(\mathcal{L}(x,y)) \neq \left[argmax_x(\int \mathcal{L}(x,y)dy), argmax_y(\int \mathcal{L}(x,y)dx)\right]$$

Proof of concept: MUonE experiment

Example of geometry optimization: **MUonE** experiment

- MUonE: high precision **muon-electron** differential cross section
  → **hadronic contributions** to **g-2 muon anomaly**

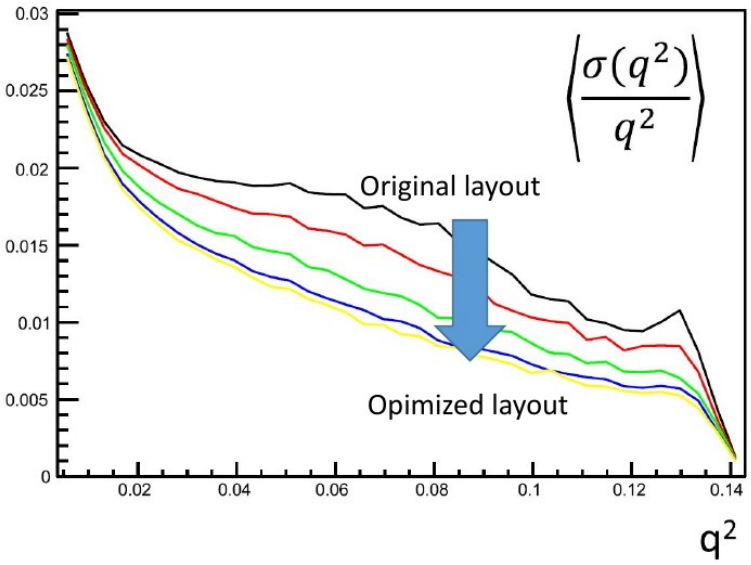




Optimizing **geometry** of the detector

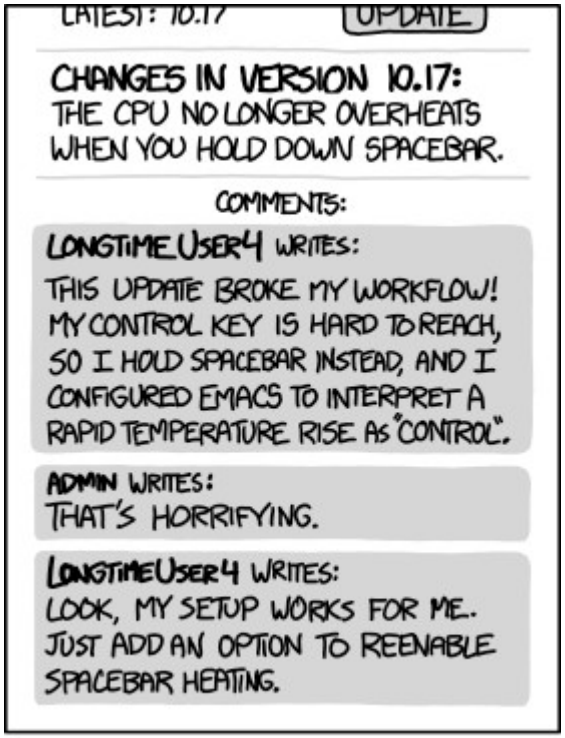
- Likelihood minimization (not autodiff.)
- **Factor 2 improvement**
- No increase of **detector cost**

Relative resolution in q^2



[T. Dorigo, https://doi.org/10.1016/j.physo.2020.100022]

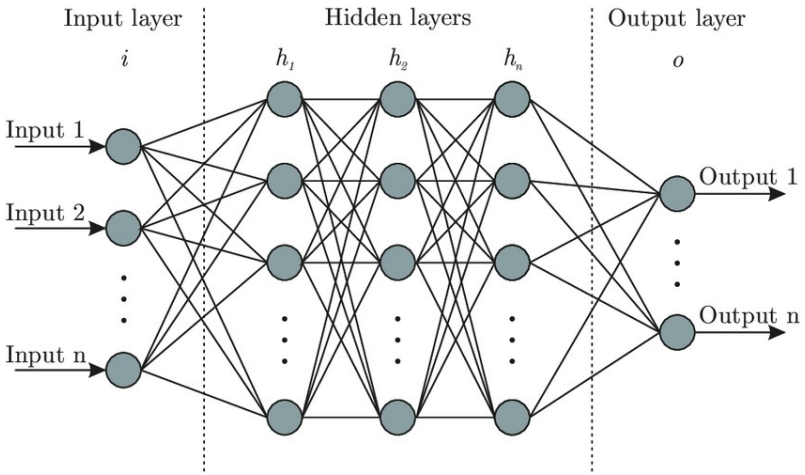
Generic optimization pipeline



EVERY CHANGE BREAKS SOMEONE'S WORKFLOW.

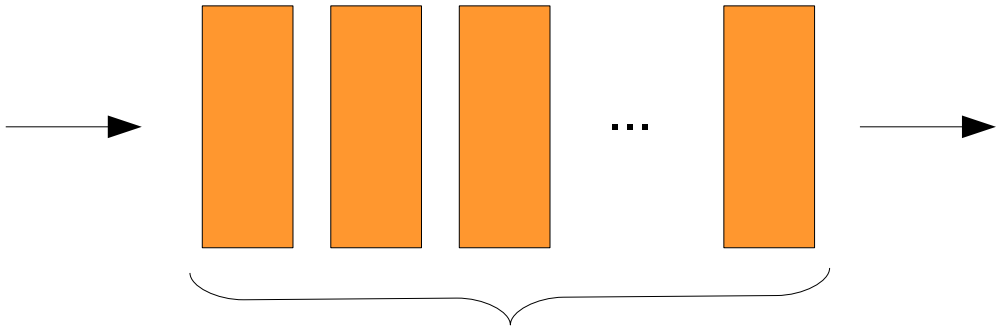
Generic optimization pipeline

Data



NN output

Data
(particles)



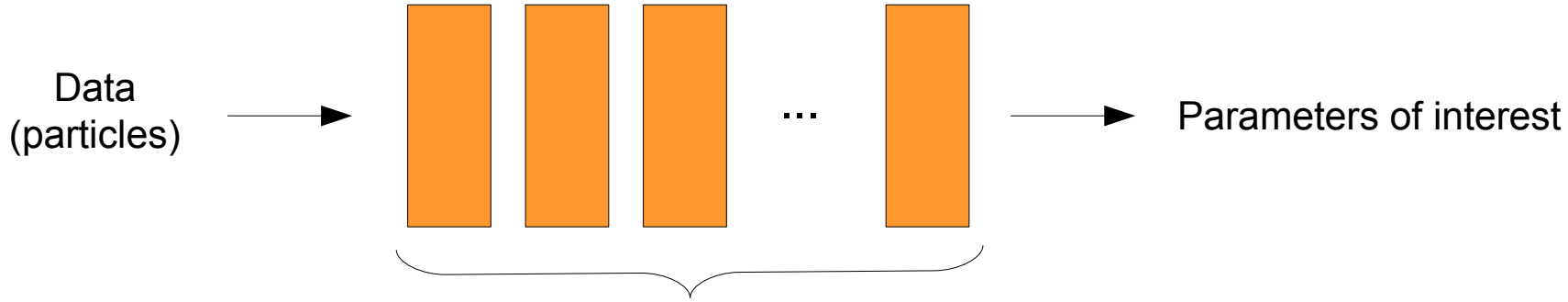
Parameters of interest

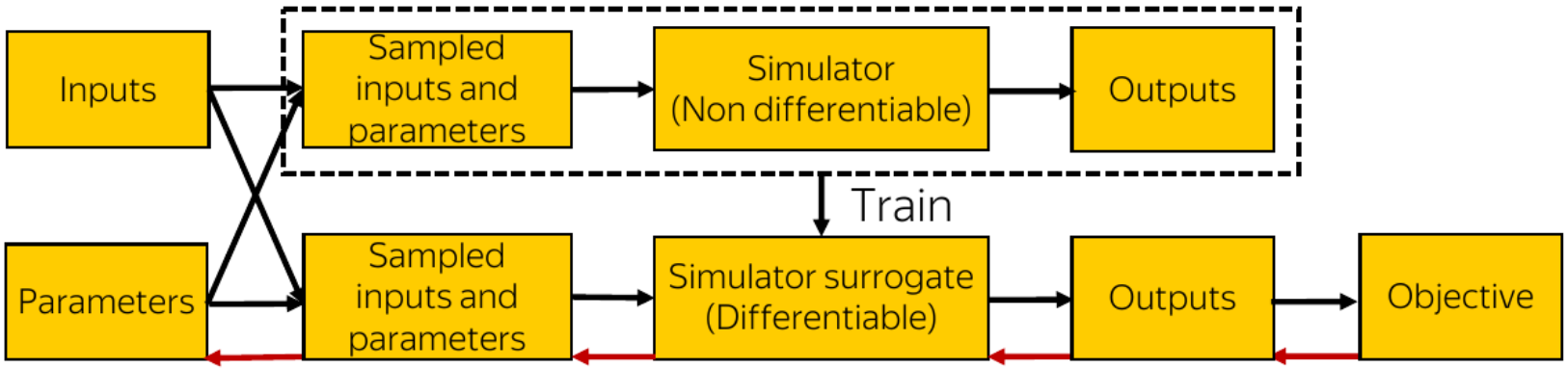
Differentiable simulated
detector **modules**

Minimization of objective function through automatic differentiation

Generic optimization pipeline

What if simulator is **not differentiable** ? Try generative **surrogate**

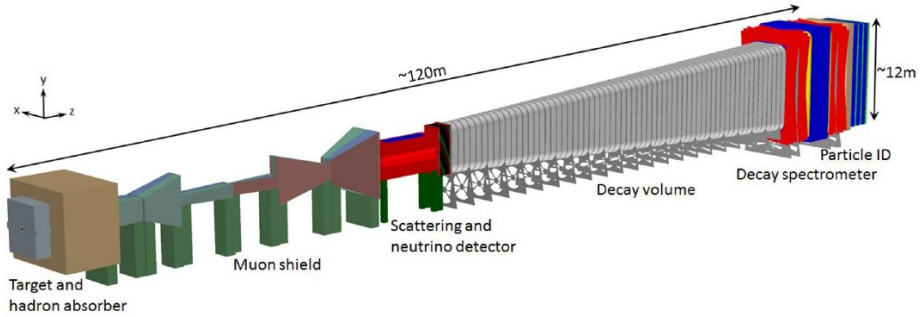




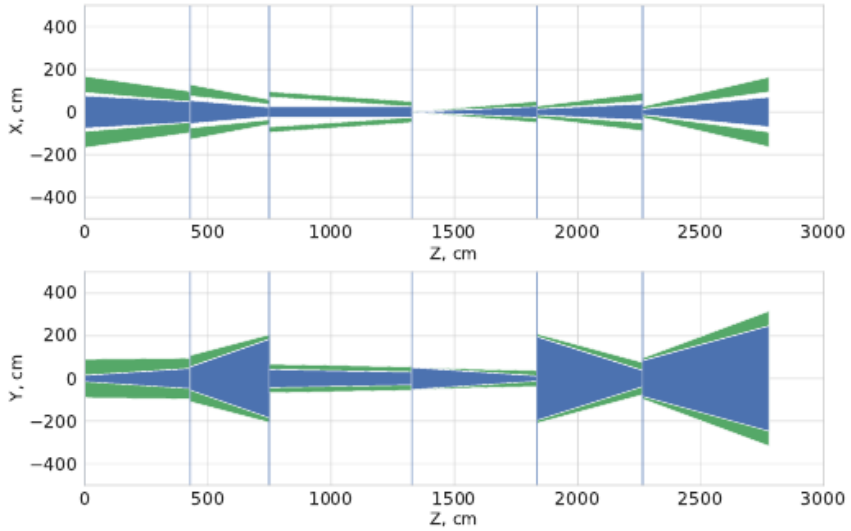
Black-Box Optimization with Local Generative Surrogates, S. Shirobokov, V. Belavin, M. Kagan, A. Ustyuzhanin, A. G. Baydin, https://arxiv.org/abs/2002.04632

Muon shielding in SHIP

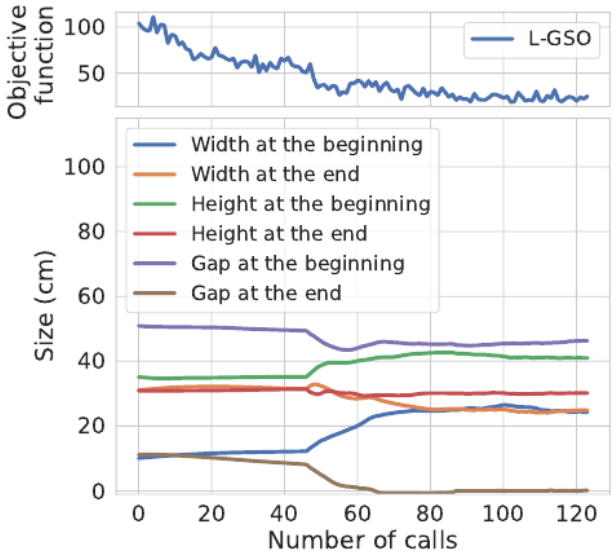
Minimize muon background fluxes in the **SHIP** steel **magnet** by varying its **geometry**



Local generative surrogate solution is **shorter** and has **lower mass** than other proposal, hence improving **efficacity** of the experiment and reducing its **cost**



Geometry of the magnet
42 parameters to optimize



Evolution of 6 parameters
during **optimization**

[2002.04632]

Machine-Learning Optimized Design of Experiments

MODE Collaboration

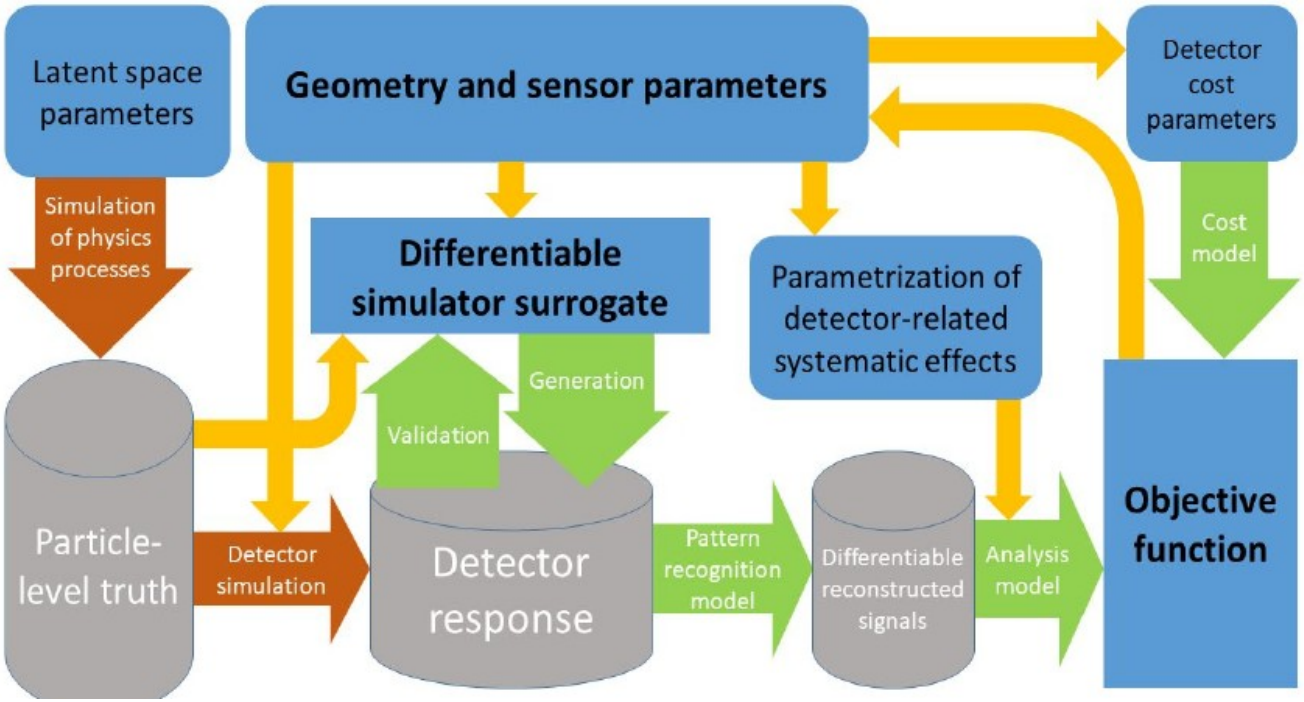
https://mode-collaboration.github.io

A. G. Baydin[5], A. Boldyrev[4], K. Cranmer[8], P. de Castro Manzano[1], T. Dorigo[1], C. Delaere[2], D. Derkach[4], J. Donini[3], A. Giammanco[2], J. Kieseler[7], G. Louppe[6], L. Layer[1], P. Martinez Ruiz del Arbol[9], F. Ratnikov[4], G. Strong[1], M. Tosi[1], A. Ustyuzhanin[4], P. Vischia[2], H. Yarar[1] + more members that joined recently

1 INFN, Sezione di Padova (and associates from Padova and Naples Universities), Italy
2 Université Catholique de Louvain, Belgium
3 Université Clermont Auvergne, France
4 Laboratory for big data analysis of the Higher School of Economics, Russia
5 University of Oxford
6 Université de Liege
7 CERN
8 New York University
9 IFCA

MODE ultimate goals

The target of **MODE** is to design and offer to the community a scalable, versatile **architecture** that can provide **end-to-end optimization of particle detectors**, proving it on a number of **different applications** across different **domains**

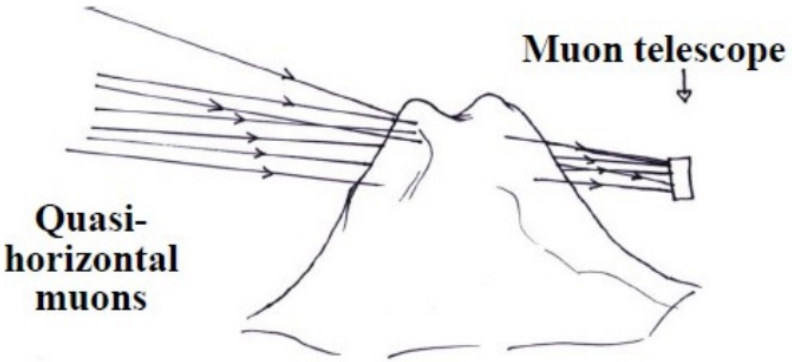


Toward Machine Learning Optimization of Experimental Design, Nuclear Physics News, 2021

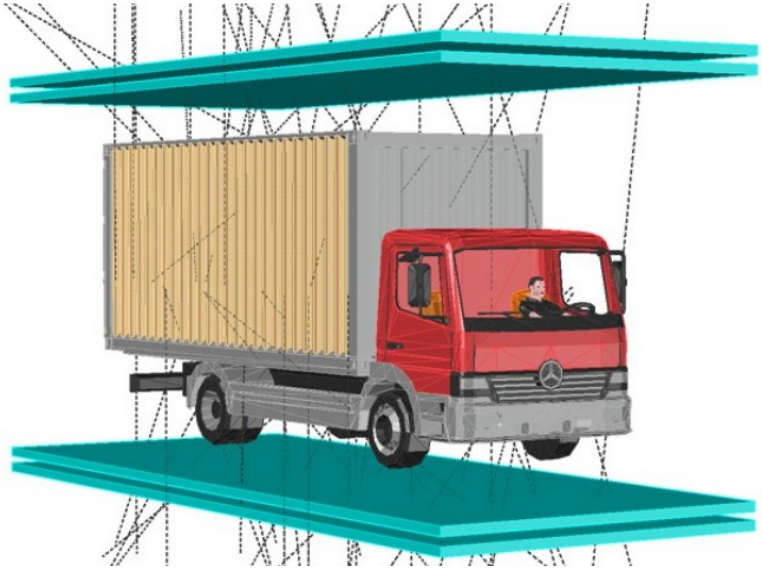
Differentiable programming for muography

Tomography: exploit **atmospheric muon** flux to **map** the interior of **objects**

Muon absorption



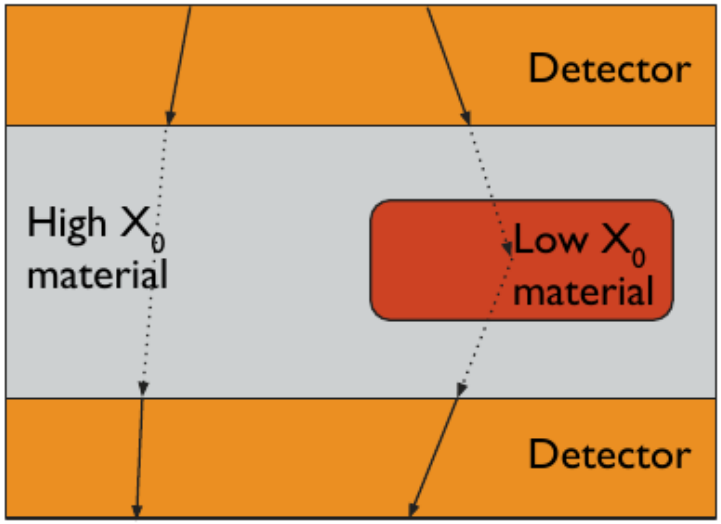
Muon scattering



[images : A. Giammanco]

Muon tomography

Volume with unknown **composition** sandwiched between **detectors**



Infer $\mathbf{X_0}$ (radiation length) of volume by measuring **muon scattering**

How should detectors be positionned for best performances ?

- i.e Muon detection **accuracy**, **resolution** on $X_{0, \ldots}$
- But also: **cost**, **size**, ...

[see G. Strong talk]

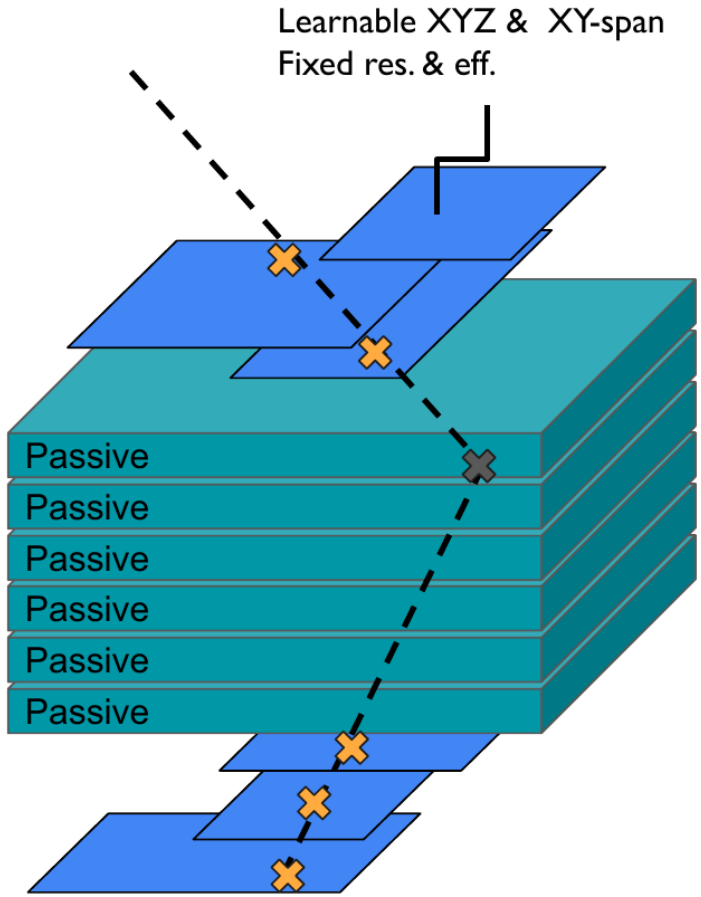
TomOpt: Tomography Optimization

Muon scan of volume of unknown density

Detector layers are regions of space containing a fixed number of panels

- Each **panel** exists and has a fixed **resolution** and **efficiency**
- The (x,y,z) **position** and xy-**span** are **parameters** to be optimised
- **Cost** of each panel scales with its area

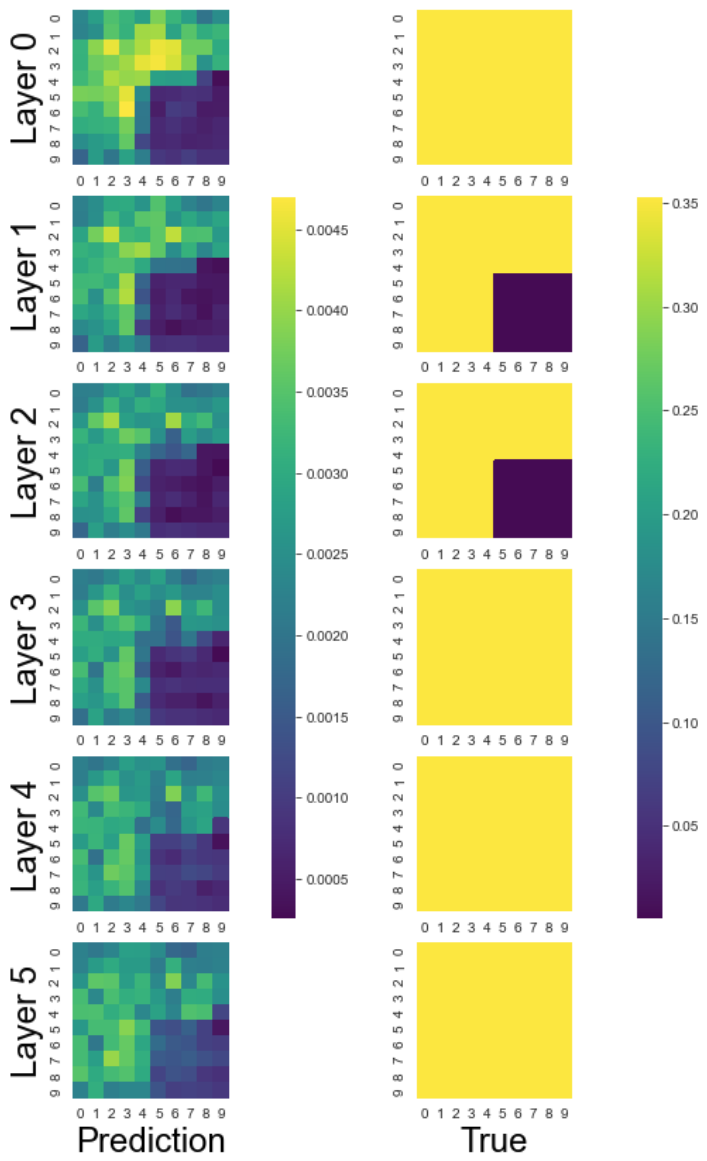
Inference is fully differentiable w.r.t. detector parameters



Python package for differential optimisation of muon-tomography detectors

G.Strong, T.Dorigo, F.Fanzago, A.Giammanco, M.Lagrange, M.Lamparth, F.Nardi, and P.Vischia

TomOpt: Tomography Optimization



Example volume

- Block of lead (X_0=0.005612m)
- Surrounded by beryllium (X_0=0.3528m)

Prediction based on 10k muons

- Lead block clearly **visible**
- The X0 predictions are **biased** due the assigning of the entirety of the muon scattering to a single point
- high **z uncertainty** in scatter location causes ‘ghosting’ above and below

[G. Strong]

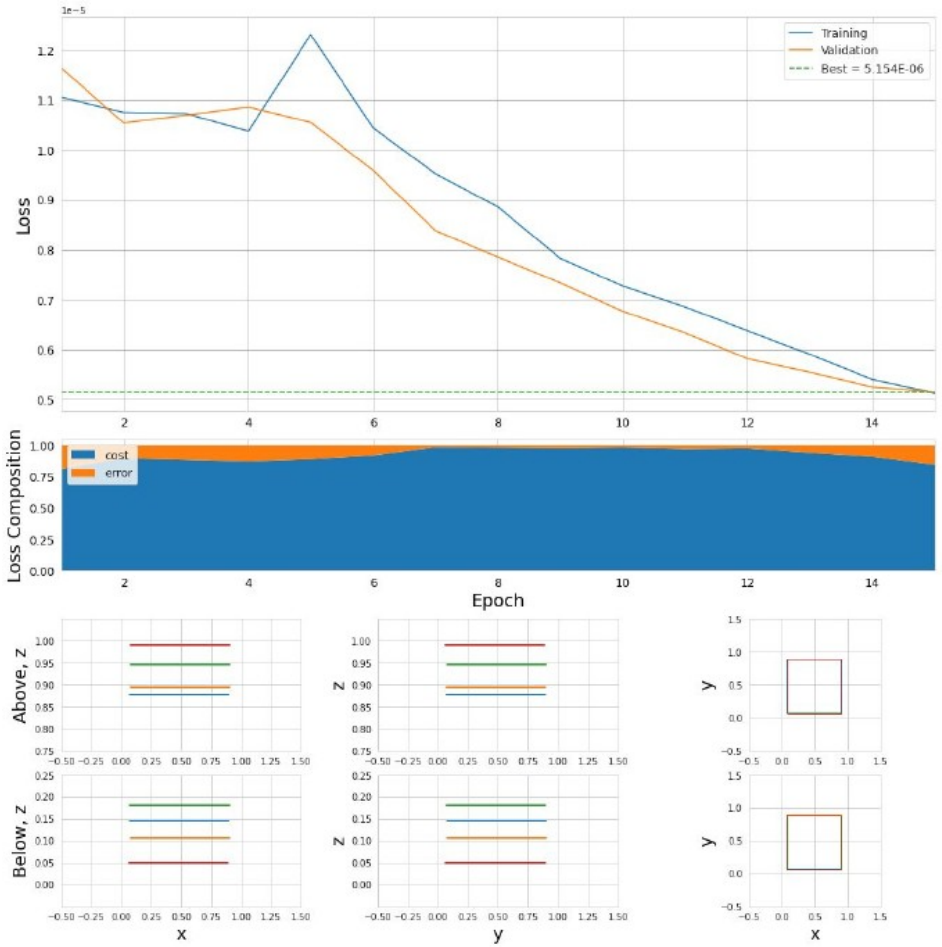
TomOpt: Tomography Optimization

Loss contains:

- Predictive performance
- And detector cost

Live **feedback** of optimisation

- Both loss and detector states



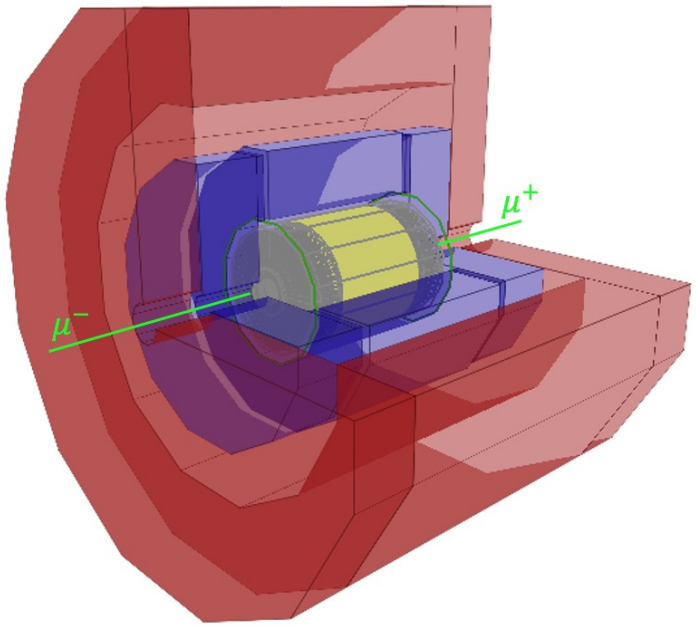
Important milestone for this use case

[G. Strong]

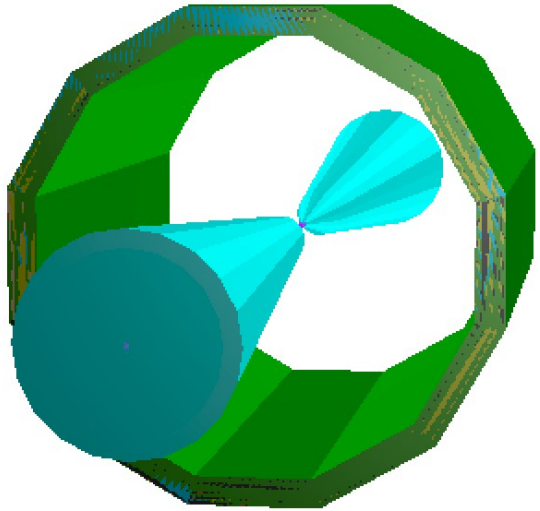
Calorimetry for Muon Collider

ECAL geometry optimization studies

- Focus on role of **Beam Induced Background** (mostly photons)
- **Mitigate** impact of BIB: granularity, segmentation, reconstruction, timing
- Aim: use Diff. Programming to **optimize geometry configuration**



Detector scheme



ECAL barrel and shielding “nozzle”

https://muoncollider.web.cern.ch/design/muon-collider-detector

Conclusion

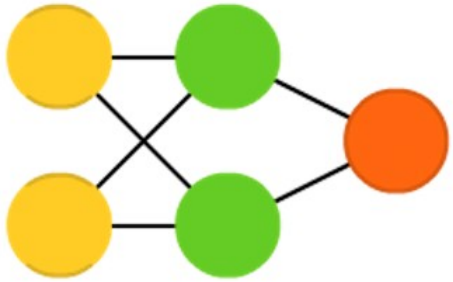
Differentiable programming paradigm opens to many different **applications**

For HEP: end-to-end **optimization** of analysis, simulators, detectors, ...

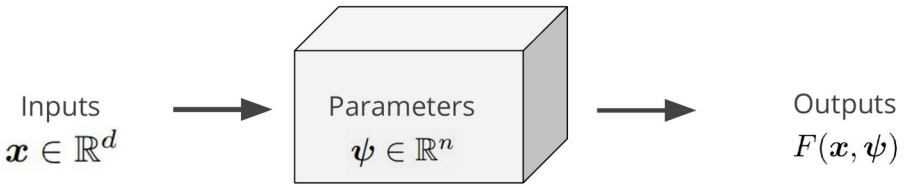
MODE collaboration: ML optimization of **detector design**

- Several **projects**: muon tomography (advanced), muon collider detector shielding (ongoing), Hybrid calorimeter (staring) + others considered
- We know this is a **challenging** and **ambitious** task !
- Objective is **not to substitute experts** in detector design
- **Domain knowledge crucial** in setting up analysis workflow
- Consider joining and bring you **use case**

Backup material

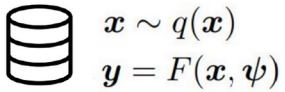


Surrogates for differentiability

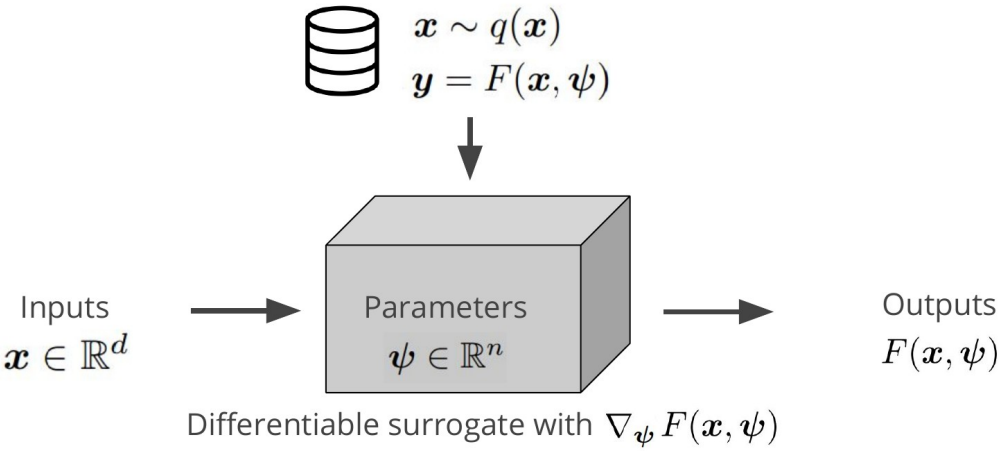


Non-differentiable simulator (model)

- Run simulator many times
- Generate a (large) dataset of input - output pairs capturing simulator's behavior



- Use the dataset to learn a differentiable approximation of the simulator (e.g., a deep generative model)



Differentiable surrogate with $\nabla_{\boldsymbol{\psi}} F(\boldsymbol{x}, \boldsymbol{\psi})$

[slides G. Baydin]

Surrogates for differentiability

Algorithm 1 Local Generative Surrogate Optimization (L-GSO) procedure

Require: number N of $\boldsymbol{\psi}$, number M of $\boldsymbol{x}$ for surrogate training, number K of $\boldsymbol{x}$ for $\boldsymbol{\psi}$ optimization step, trust region U_ϵ, size of the neighborhood ϵ, Euclidean distance d

1: Choose initial parameter $\boldsymbol{\psi}$
2: **while** $\boldsymbol{\psi}$ has not converged **do**
3: Sample $\boldsymbol{\psi}_i$ in the region $U_\epsilon^{\boldsymbol{\psi}},\ i = 1, \ldots, N$
4: For each $\boldsymbol{\psi}_i$, sample inputs $\{\boldsymbol{x}_j^i\}_{j=1}^M \sim q(\boldsymbol{x})$
5: Sample $M \times N$ training examples from simulator $\boldsymbol{y}_{ij} = F(\boldsymbol{x}_j^i; \boldsymbol{\psi}_i)$
6: Store $\boldsymbol{y}_{ij}, \boldsymbol{x}_j^i, \boldsymbol{\psi}_i$ in history H $i = 1, \ldots, N; j = 1, \ldots, M$
7: Extract all $\boldsymbol{y}_l, \boldsymbol{x}_l, \boldsymbol{\psi}_l$ from history H, iff $d(\boldsymbol{\psi}, \boldsymbol{\psi}_l) < \epsilon$
8: Train generative surrogate model $S_\theta(\boldsymbol{z}_l, \boldsymbol{x}_l; \boldsymbol{\psi}_l)$, where $\boldsymbol{z}_l \sim \mathcal{N}(0, 1)$
9: Fix weights of the surrogate model θ
10: Sample $\bar{\boldsymbol{y}}_k = S_\theta(\boldsymbol{z}_k, \boldsymbol{x}_k; \boldsymbol{\psi}), \boldsymbol{z}_k \sim \mathcal{N}(0, 1)$, $\boldsymbol{x}_k \sim q(\boldsymbol{x}),\ k = 1, \ldots, K$
11: $\nabla_{\boldsymbol{\psi}}\, \mathbb{E}[\mathcal{R}(\bar{\boldsymbol{y}})] \leftarrow \frac{1}{K} \sum_{k=1}^{K} \frac{\partial \mathcal{R}}{\partial \bar{\boldsymbol{y}}_k} \frac{\partial S_\theta(\boldsymbol{z}_k, \boldsymbol{x}_k; \boldsymbol{\psi})}{\partial \boldsymbol{\psi}}$
12: $\boldsymbol{\psi} \leftarrow \mathrm{SGD}(\psi, \nabla_{\boldsymbol{\psi}}\, \mathbb{E}[\mathcal{R}(\bar{\boldsymbol{y}})])$
13: **end while**

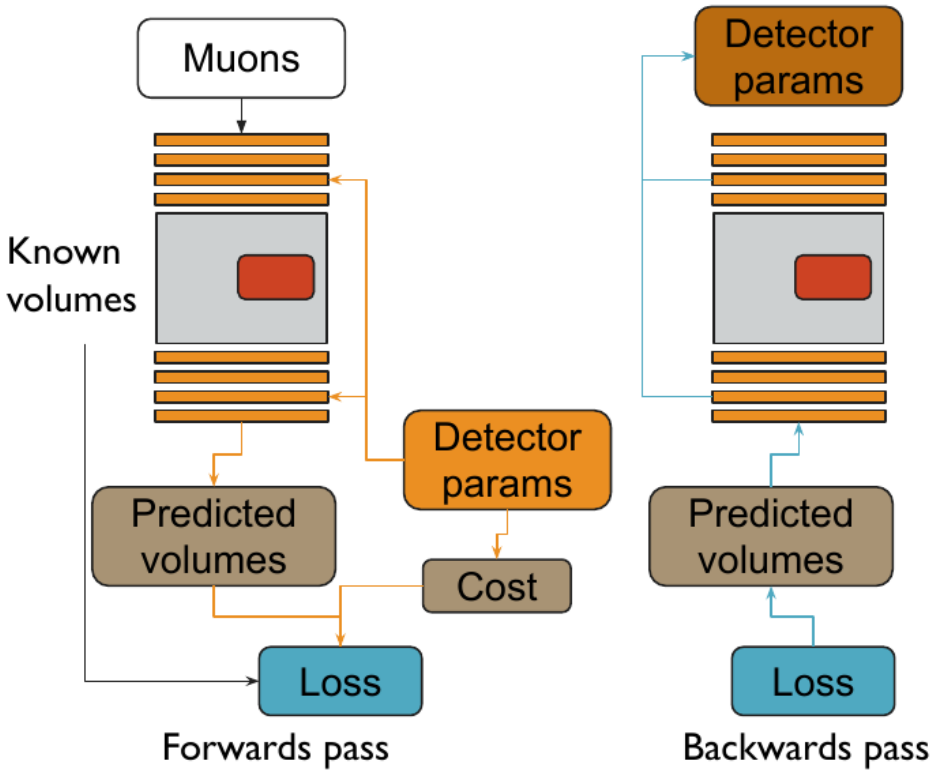
$$\boldsymbol{\psi}^* = \arg\min_{\boldsymbol{\psi}} \mathbb{E}[\mathcal{R}(\boldsymbol{y})] = \arg\min_{\boldsymbol{\psi}} \int \mathcal{R}(\boldsymbol{y}) p(\boldsymbol{y}|\boldsymbol{x}; \boldsymbol{\psi}) q(\boldsymbol{x}) d\boldsymbol{x} d\boldsymbol{y}$$

$$\approx \arg\min_{\boldsymbol{\psi}} \frac{1}{N} \sum_{i=1}^{N} \mathcal{R}(F(\boldsymbol{x}_i; \boldsymbol{\psi}))$$

$$\nabla_{\boldsymbol{\psi}}\, \mathbb{E}[\mathcal{R}(\boldsymbol{y})] \approx \frac{1}{N} \sum_{i=1}^{N} \nabla_{\boldsymbol{\psi}} \mathcal{R}(S_\theta(\boldsymbol{z}_i, \boldsymbol{x}_i; \boldsymbol{\psi}))$$

TomOpt: end-to-end optimization

- Consider instead simulating muon propagation and expressing the entire inference chain as a differentiable system
  - We can now compute the analytical effects of detector parameters (position, size, resolution, etc.) on system outputs
- Now express the desired task as a loss function
  - E.g. error on X_0 predictions, detector costs, time to achieve desired resolution
- We can now backpropagate the loss gradient to detector parameters and optimise via gradient descent
  - Just like a neural network



[G. Strong talk]

Joining MODE ?

If you are doing experimental research in HEP, astro-HEP, neutrino physics, or high-energy nuclear physics, or if you are working at spin-offs involving, *e.g.,* muon tomography, hadron therapy, or other endeavours which operate with instruments that extract information from the interaction of energetic radiation with matter, you are very likely to have a use case – a system liable to benefit from a study with differentiable programming.

The idea of MODE is to bring together ML experts who are developing the interfaces for these applications, with the researchers who have problems to solve in their area of interest

We cannot offer a solution to any given problem (we lack the manpower to work on-demand), but together we may work toward it

☐ **Consider joining MODE, and bring your use case!**

Do I have a use case checklist:

Are you involved in the design, assembly, or upgrade of an instrument?

Can you specify one or a set of desirable scientific goals from its use?

Are those goals achieved through information processing?

If your answers to all are «yes», **you have something to optimize** and chances are this can't be done without a deep learning model of the full information extraction chain.

[slide T. Dorigo]

Muon collider detector

hadronic calorimeter

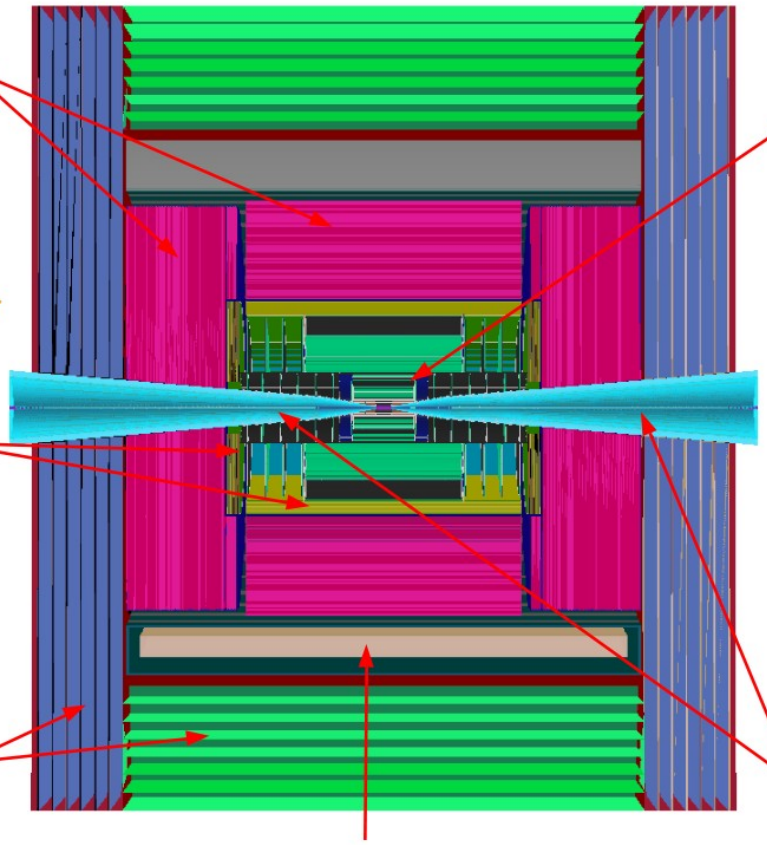
- 60 layers of 19-mm steel absorber + plastic scintillating tiles;
- 30x30 mm^2 cell size;
- 7.5 λ_I.

electromagnetic calorimeter

- 40 layers of 1.9-mm W absorber + silicon pad sensors;
- 5x5 mm^2 cell granularity;
- 22 X_0 + 1 λ_I.

muon detectors

- 7-barrel, 6-endcap RPC layers interleaved in the magnet's iron yoke;
- 30x30 mm^2 cell size.



superconducting solenoid (3.57T)

tracking system

- Vertex Detector:
  - double-sensor layers (4 barrel cylinders and 4+4 endcap disks);
  - 25x25 μm^2 pixel Si sensors.
- Inner Tracker:
  - 3 barrel layers and 7+7 endcap disks;
  - 50 µm x 1 mm macro-pixel Si sensors.
- Outer Tracker:
  - 3 barrel layers and 4+4 endcap disks;
  - 50 µm x 10 mm micro-strip Si sensors.

shielding nozzles

- Tungsten cones + borated polyethylene cladding.

https://muoncollider.web.cern.ch/design/muon-collider-detector