InvertibleNetworks.jl – Memory efficient deep learning in Julia

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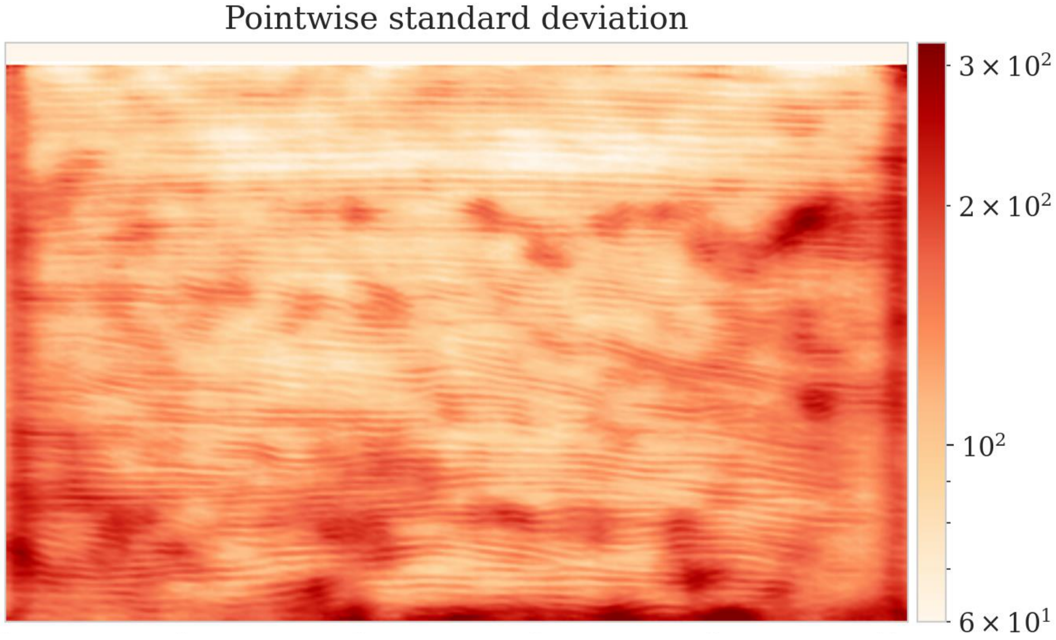
Seismic Laboratory for Imaging and Modeling

Invertible Neural Networks

(Kingma & Dhariwal, 2018)

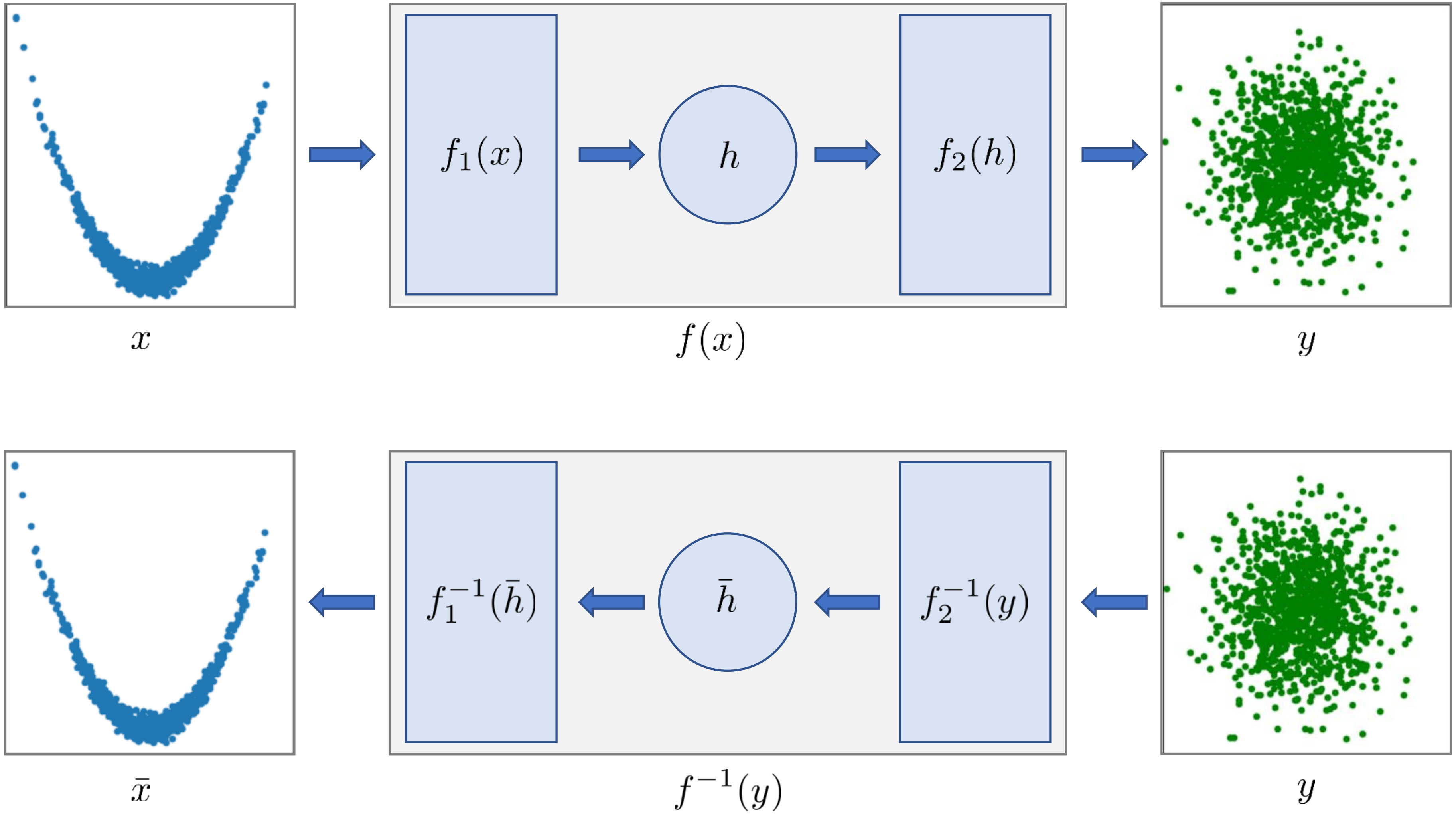
Generative Modeling via Normalizing Flows



(Siahkoohi et al., 2021)

Inverse problems & Uncertainty quantification (UQ)

Invertible Neural Networks



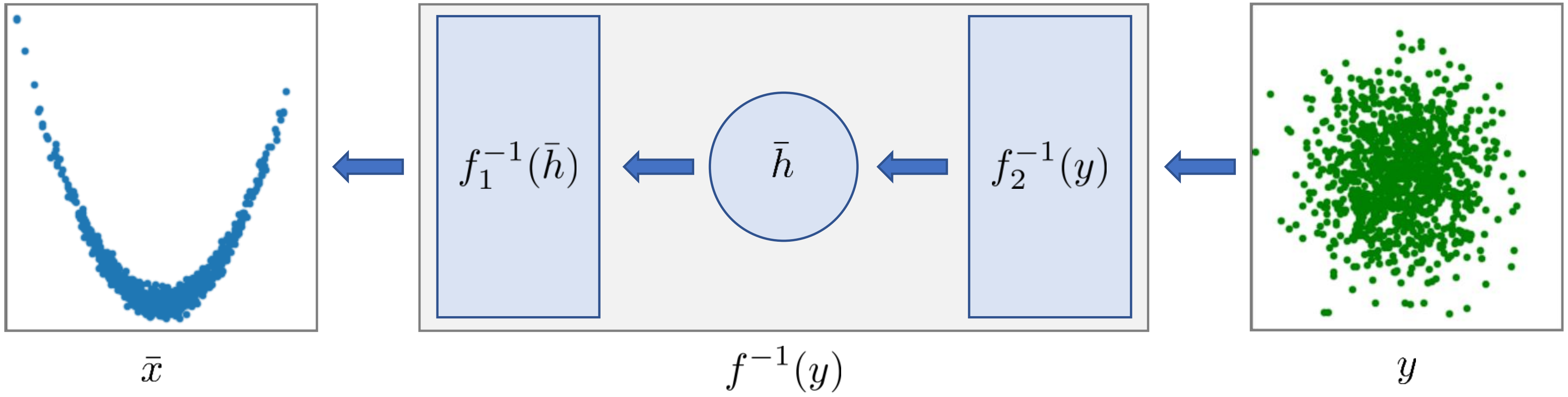
$f_1(x)$ → h → $f_2(h)$

x | $f(x)$ | y

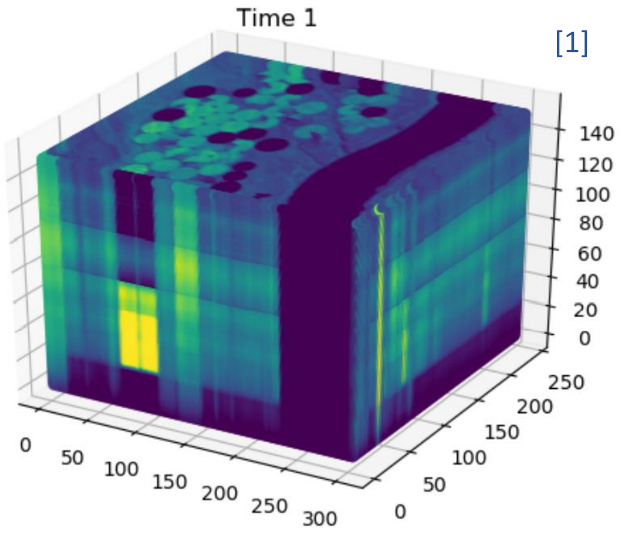
$f_1^{-1}(\bar{h})$ ← $\bar{h}$ ← $f_2^{-1}(y)$

$\bar{x}$ | $f^{-1}(y)$ | y

Invertible Neural Networks



- Train deep 3D neural networks
  - Take advantage of invertibility
  - No need to store hidden states



[1]

[1] Peters et al., Fully reversible neural networks for large-scale surface and sub-surface characterization via remote sensing. arXiv preprints, 2020.

INN & NF frameworks

- Relevant Julia packages
  - Flux.jl [1]
  - Knet.jl [2]
  - Bijections.jl [3]
  - No specific INN & NF frameworks

→ **No frameworks that optimally take advantage of invertibility**

- Python packages
  - Frameworks for Easily Invertible Architectures (FrEIA) [4]
  - MemCNN [5]
  - PyTorch Normalizing Flows [6]

- Papers with code
  - Glow [7]
  - Invertible RIM + Fast MRI [8]
  - Invertible Residual Networks [9]
  - Etc.

[1] Innes, Mike. *Flux: Elegant Machine Learning with Julia*, Journal of Open Source Software, 2018

[2] Yuret, Deniz. *Knet: Beginning deep learning with 100 lines of Julia.* Machine Learning Systems Workshop, NeurIPS, 2016

[3] Scheinerman et al., *Bijections.jl.* https://github.com/scheinerman/Bijections.jl, 2021

[4] Kruse et al., *FrEIA*. https://github.com/VLL-HD/FrEIA, 2021

[5] Van de Leemput et al. *MemCNN: A Python/PyTorch package for creating memory-efficient INNs*, Journal of Open Source Software, 2019

[6] Karpathy, Andrew. *PyTorch Normalizing Flows*. https://github.com/karpathy/pytorch-normalizing-flows, 2019.

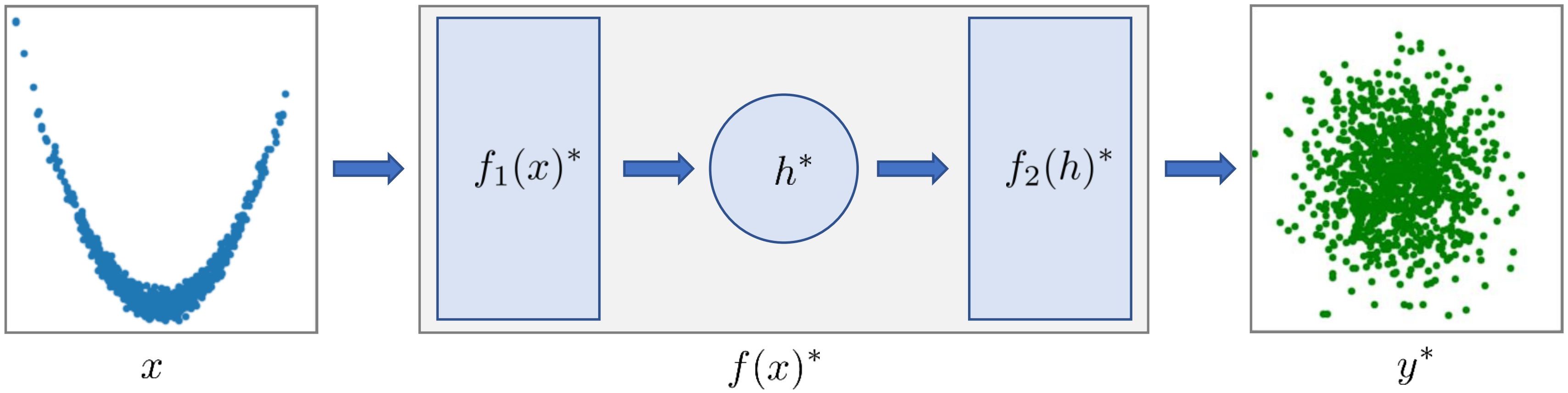
[7] Kingma & Dhariwal. *Glow: Generative Flow with Invertible 1x1 Convolutions*. arXiv preprints, 2018.

[8] Putzky et al. *i-RIM applied to the fastMRI challenge*. ariXiv preprints, 2019.

[9] Behrmann et al. *Invertible Residual Networks*. ICML, 2019.

Training INNs & NFs

Forward pass

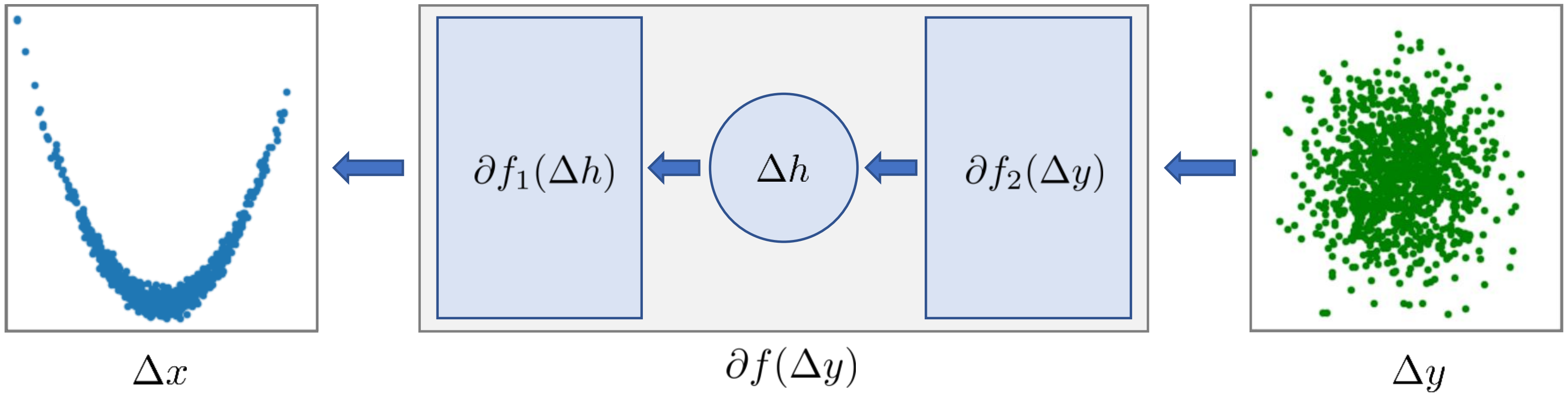


$f_1(x)^*$ → h^* → $f_2(h)^*$

x → $f(x)^*$ → y^*

* tracked

Backprop with AD

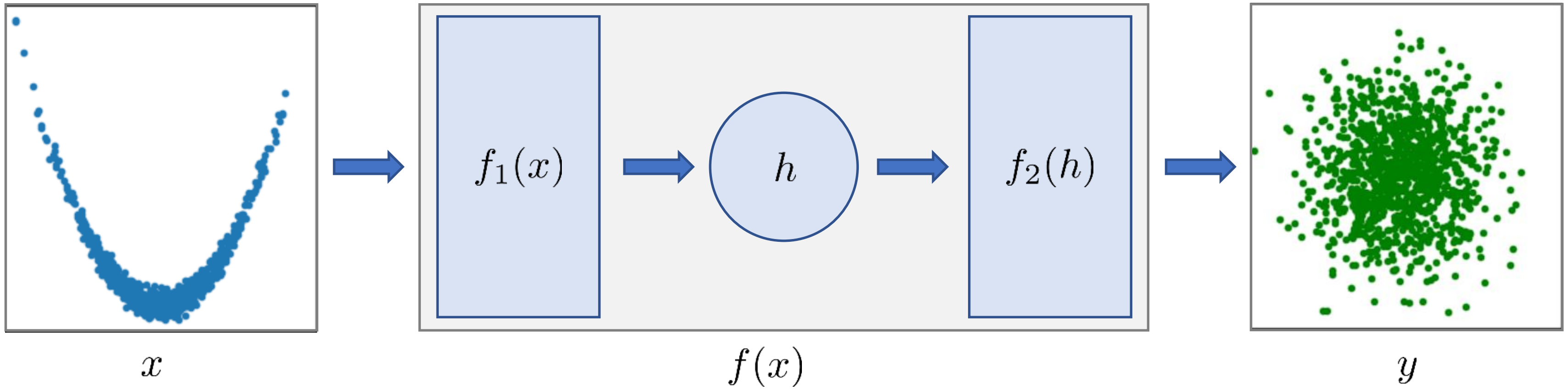


$\partial f_1(\Delta h)$ ← Δh ← $\partial f_2(\Delta y)$

Δx ← $\partial f(\Delta y)$ ← Δy

Training INNs & NFs

Forward pass

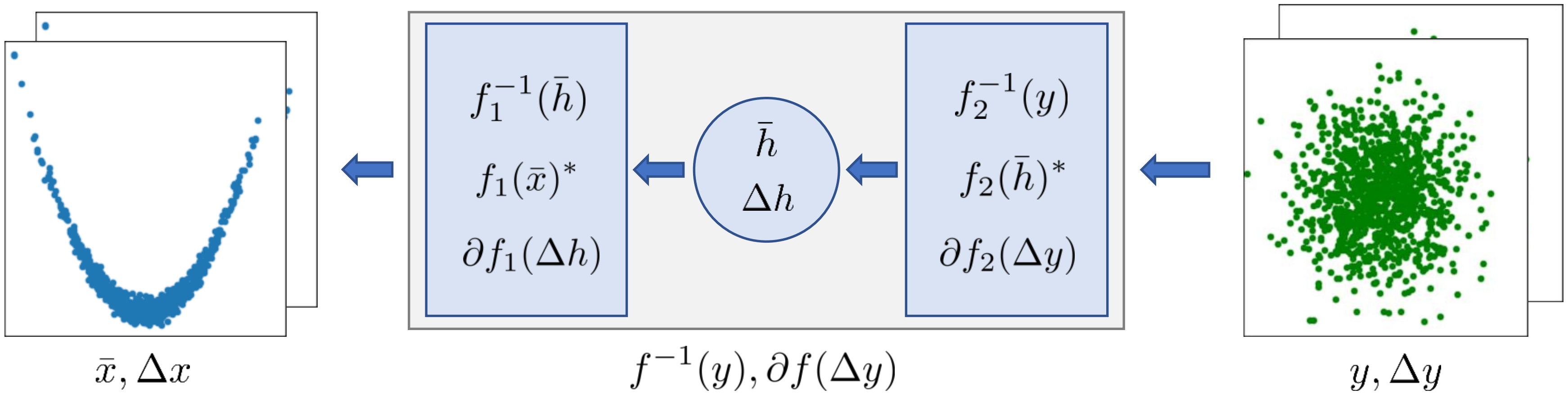


$f_1(x)$ → h → $f_2(h)$

x $f(x)$ y

(no tracking)

Backprop layer-wise AD



$f_1^{-1}(\bar{h})$

$f_1(\bar{x})^*$

$\partial f_1(\Delta h)$

$\bar{h}$

Δh

$f_2^{-1}(y)$

$f_2(\bar{h})^*$

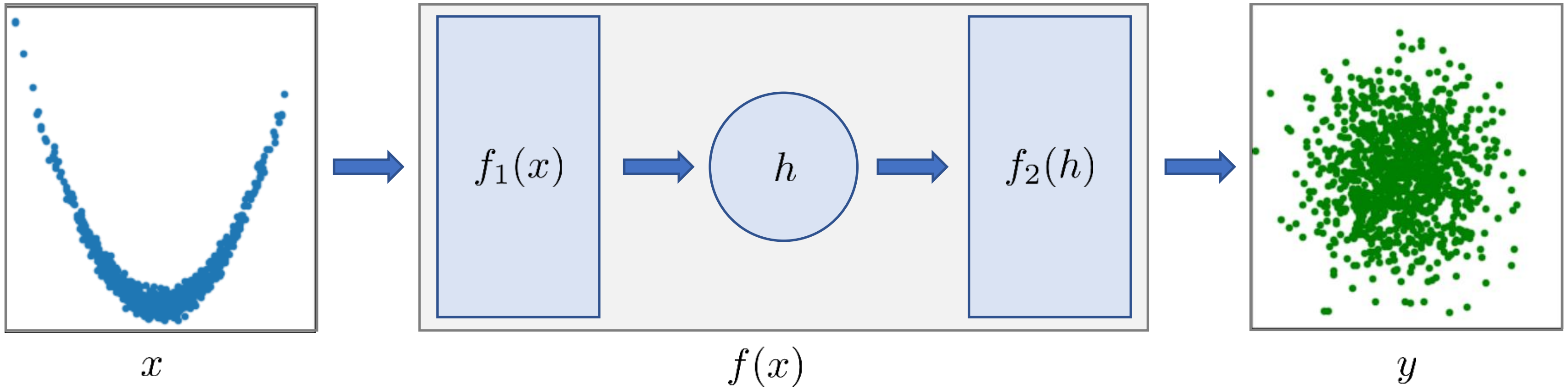
$\partial f_2(\Delta y)$

$\bar{x}, \Delta x$ $f^{-1}(y), \partial f(\Delta y)$ $y, \Delta y$

* tracked

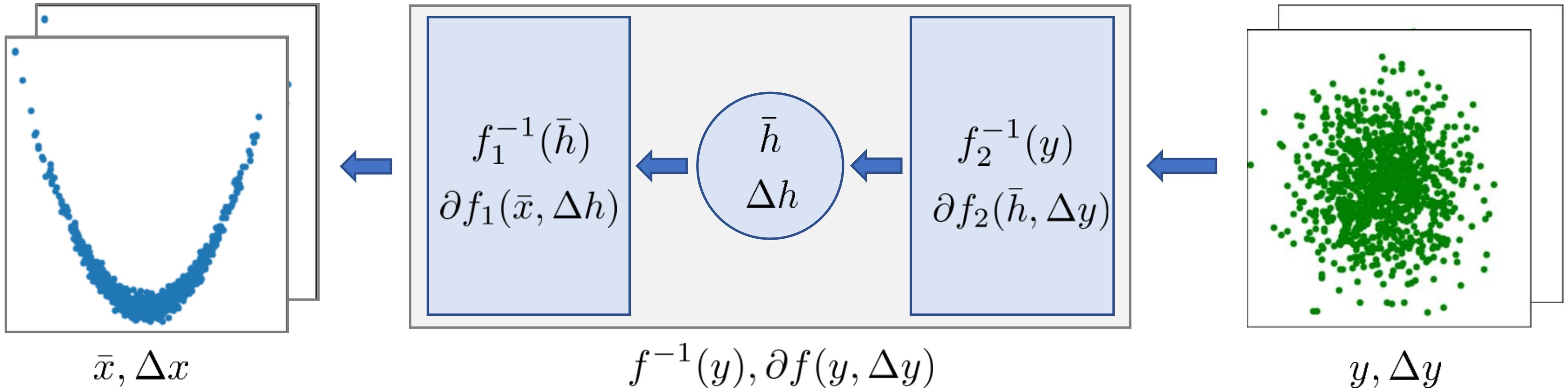
Training INNs & NFs

Forward pass



(no tracking)

Backprop no AD



(no tracking,
no extra forward pass)

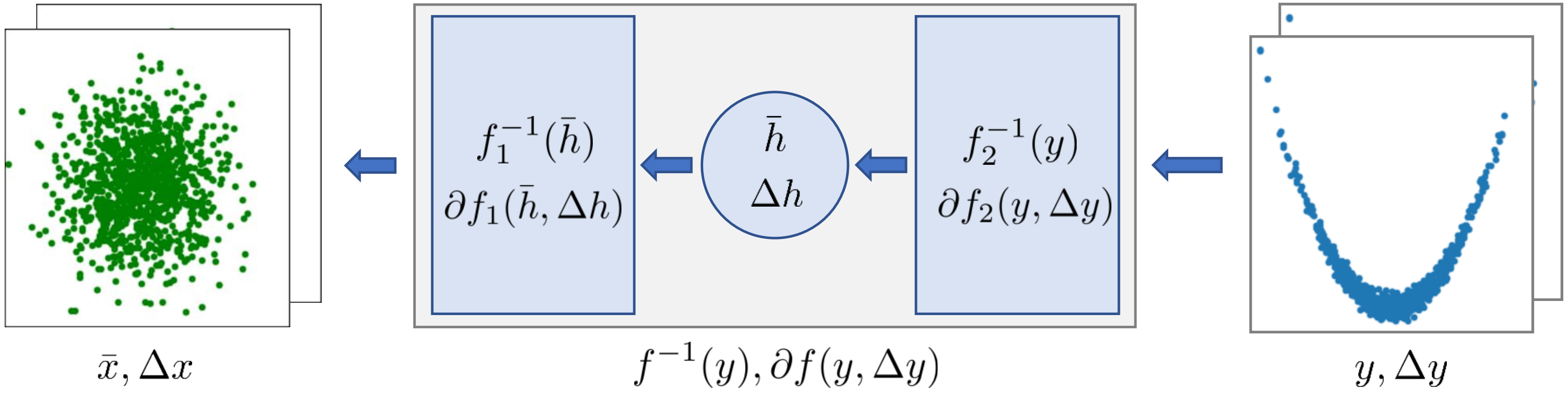
[1] Kruse et al., *HINT: Hierarchical Invertible Neural Transport for Density Estimation and Bayesian Inference*. Proceedings of AAAI, 2021

[2] Putzky et al. *i-RIM applied to the fastMRI challenge*. ariXiv preprints, 2019.

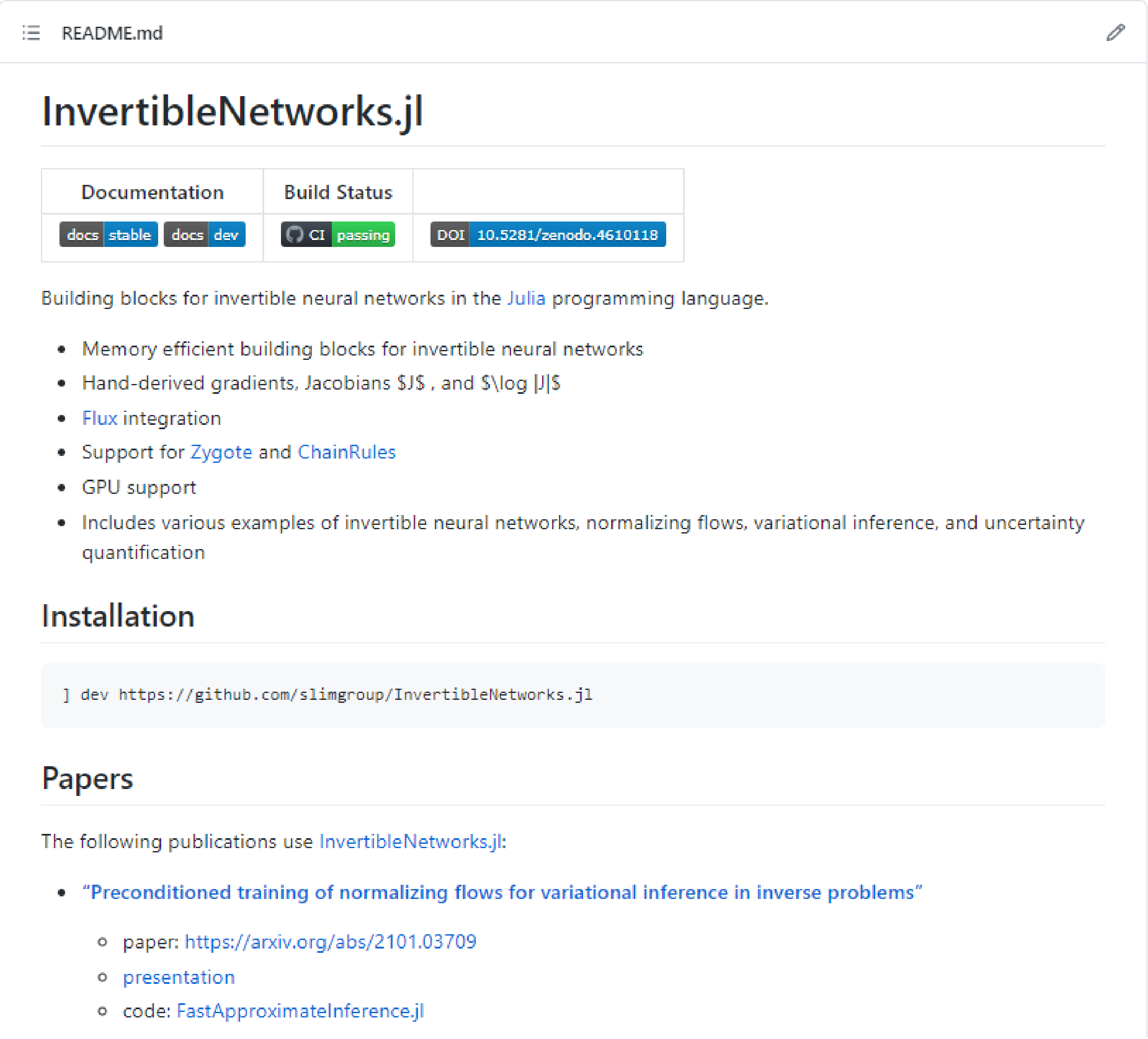
[3] Kingma & Dhariwal. *Glow: Generative Flow with Invertible 1x1 Convolutions*. arXiv preprints, 2018.

InvertibleNetworks.jl

- Memory efficient training for INNs & NFs (MIT license)



- Common building blocks from literature
  - Coupling layers, hyperbolic layers, i-RIM, HINT, 1 x 1 convolutions, etc. [1-3]
  - Log-dets for training via change of variables
  - Forward + adjoint Jacobians (forward + backward differentiation)



README.md

InvertibleNetworks.jl

Documentation	Build Status	
docs stable docs dev	CI passing	DOI 10.5281/zenodo.4610118

Building blocks for invertible neural networks in the Julia programming language.

- Memory efficient building blocks for invertible neural networks
- Hand-derived gradients, Jacobians J , and $\log |J|$
- Flux integration
- Support for Zygote and ChainRules
- GPU support
- Includes various examples of invertible neural networks, normalizing flows, variational inference, and uncertainty quantification

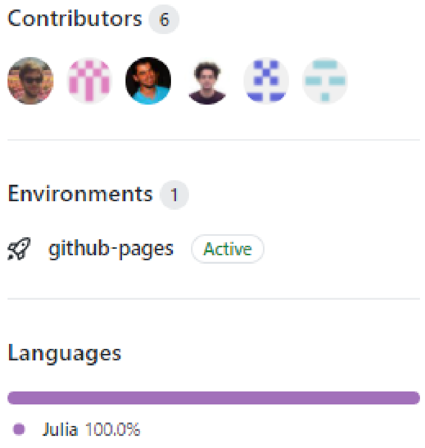
Installation

```
] dev https://github.com/slimgroup/InvertibleNetworks.jl
```

Papers

The following publications use InvertibleNetworks.jl:

- “Preconditioned training of normalizing flows for variational inference in inverse problems”
  - paper: https://arxiv.org/abs/2101.03709
  - presentation
  - code: FastApproximateInference.jl



Contributors 6

Environments 1

github-pages Active

Languages

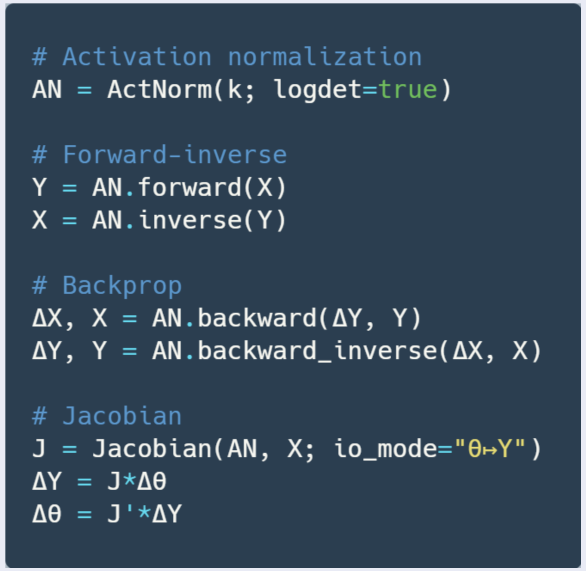
Julia 100.0%

Github repository (MIT license)

https://github.com/slimgroup/InvertibleNetworks.jl

Package overview

Invertible layers	Invertible networks	Utilities	Examples
• Coupling layers (affine, additive, Glow, HINT) • Hyperbolic layers • Activation normalization • 1 x 1 convolutions w/ Householder matrices • Log-dets for NFs	• Glow • Hyperbolic networks • HINT • i-RIM	• Activations • Dimensionality operations (squeeze, checkerboard, wavelet transform) • Objective functions • Log-dets	• Generative models • Seismic imaging/inversion • Image segmentation • Loop unrolling for inverse problems

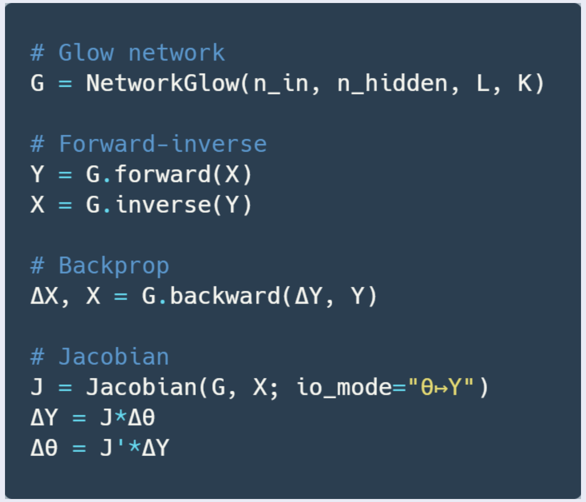


```
# Activation normalization
AN = ActNorm(k; logdet=true)

# Forward-inverse
Y = AN.forward(X)
X = AN.inverse(Y)

# Backprop
ΔX, X = AN.backward(ΔY, Y)
ΔY, Y = AN.backward_inverse(ΔX, X)

# Jacobian
J = Jacobian(AN, X; io_mode="θ↔Y")
ΔY = J*Δθ
Δθ = J'*ΔY
```



```
# Glow network
G = NetworkGlow(n_in, n_hidden, L, K)

# Forward-inverse
Y = G.forward(X)
X = G.inverse(Y)

# Backprop
ΔX, X = G.backward(ΔY, Y)

# Jacobian
J = Jacobian(G, X; io_mode="θ↔Y")
ΔY = J*Δθ
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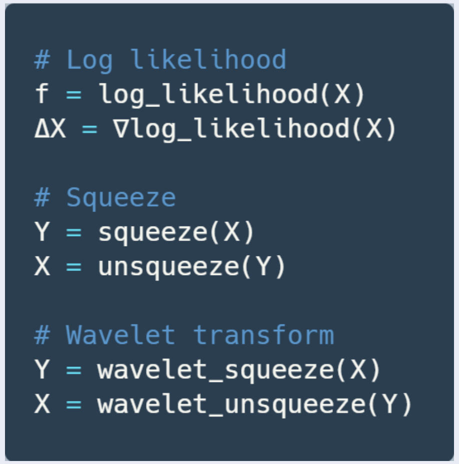
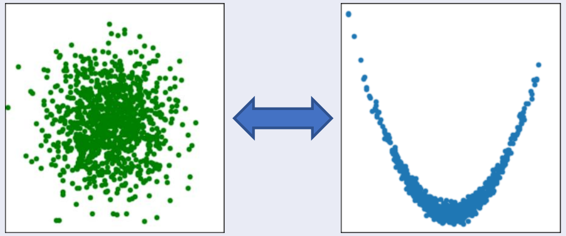
```



```
# Log likelihood
f = log_likelihood(X)
ΔX = ∇log_likelihood(X)

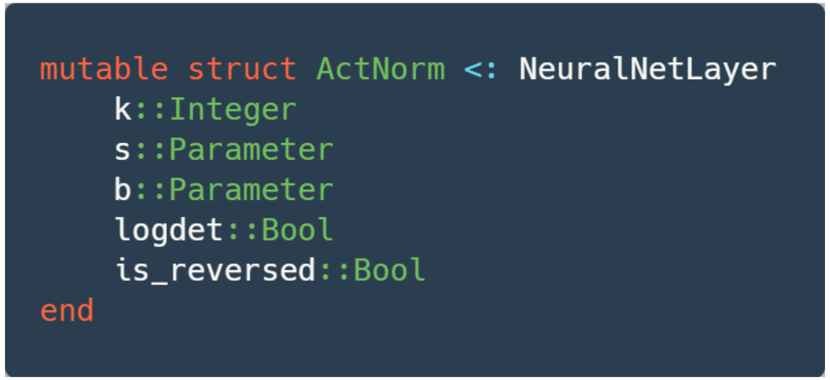
# Squeeze
Y = squeeze(X)
X = unsqueeze(Y)

# Wavelet transform
Y = wavelet_squeeze(X)
X = wavelet_unsqueeze(Y)
```



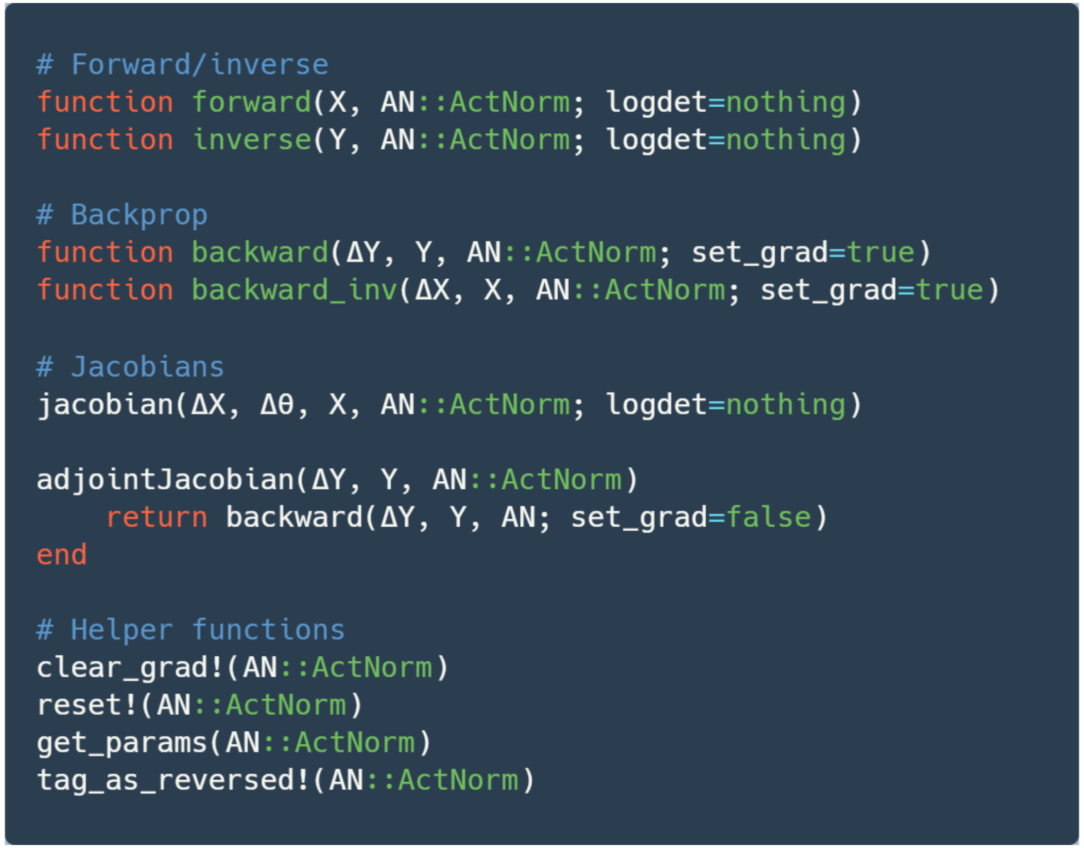
Architecture

- Each layer is mutable structure with associated methods



```
mutable struct ActNorm <: NeuralNetLayer
    k::Integer
    s::Parameter
    b::Parameter
    logdet::Bool
    is_reversed::Bool
end
```

Code structure of invertible layers



```
# Forward/inverse
function forward(X, AN::ActNorm; logdet=nothing)
function inverse(Y, AN::ActNorm; logdet=nothing)

# Backprop
function backward(ΔY, Y, AN::ActNorm; set_grad=true)
function backward_inv(ΔX, X, AN::ActNorm; set_grad=true)

# Jacobians
jacobian(ΔX, Δθ, X, AN::ActNorm; logdet=nothing)

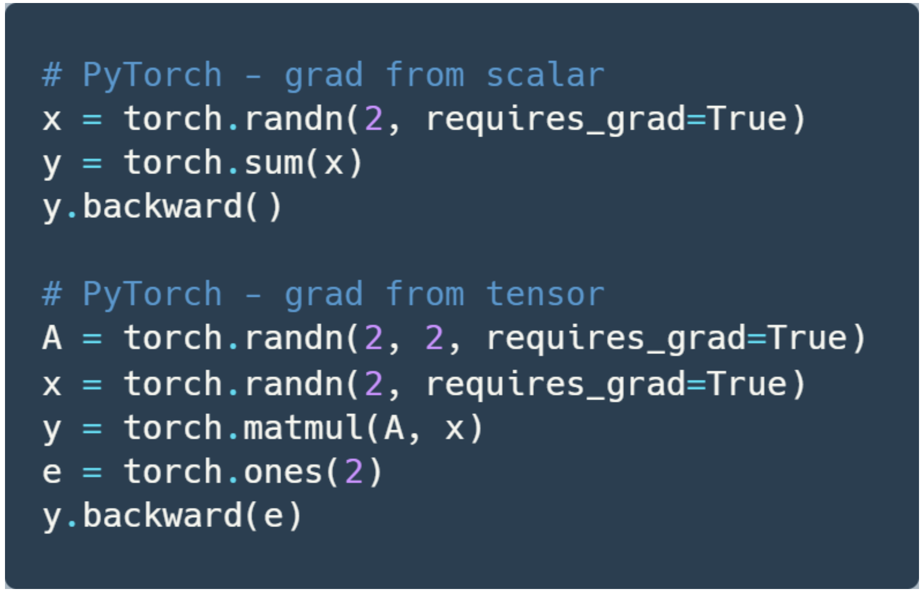
adjointJacobian(ΔY, Y, AN::ActNorm)
    return backward(ΔY, Y, AN; set_grad=false)
end

# Helper functions
clear_grad!(AN::ActNorm)
reset!(AN::ActNorm)
get_params(AN::ActNorm)
tag_as_reversed!(AN::ActNorm)
```

Gradients & Jacobians

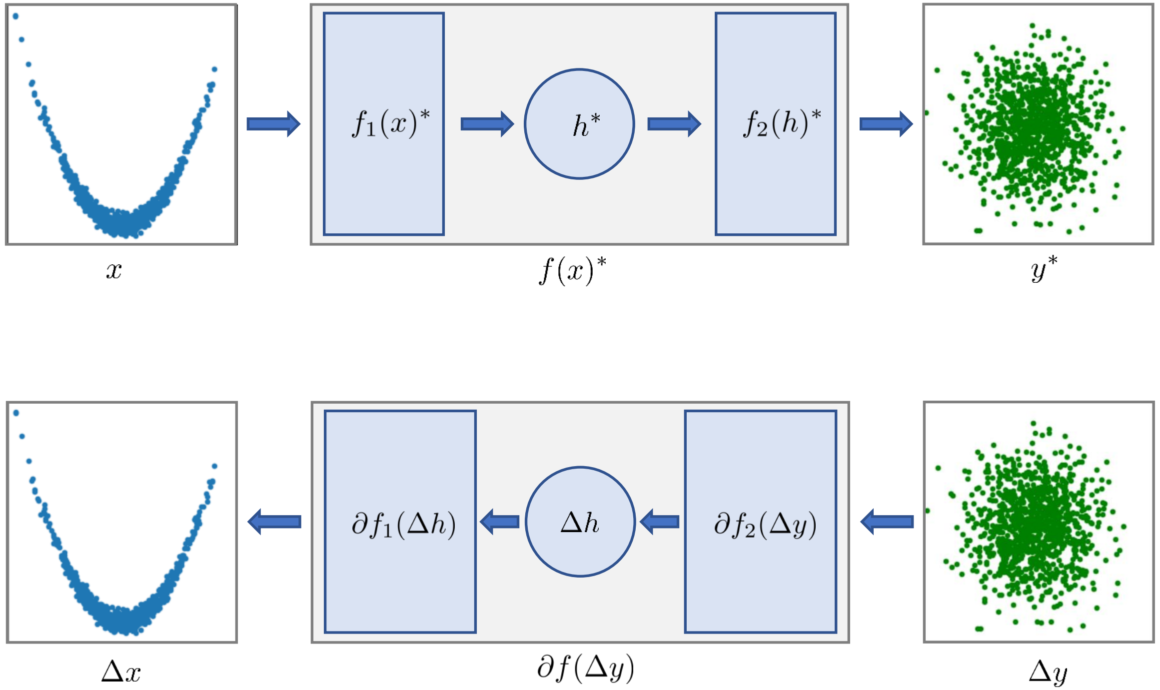
PyTorch Autograd

- Does not take original input as argument
- Input tracked during forward pass
- Same for TensorFlow, Flux, etc.



```
# PyTorch - grad from scalar
x = torch.randn(2, requires_grad=True)
y = torch.sum(x)
y.backward()

# PyTorch - grad from tensor
A = torch.randn(2, 2, requires_grad=True)
x = torch.randn(2, requires_grad=True)
y = torch.matmul(A, x)
e = torch.ones(2)
y.backward(e)
```



Gradients & Jacobians

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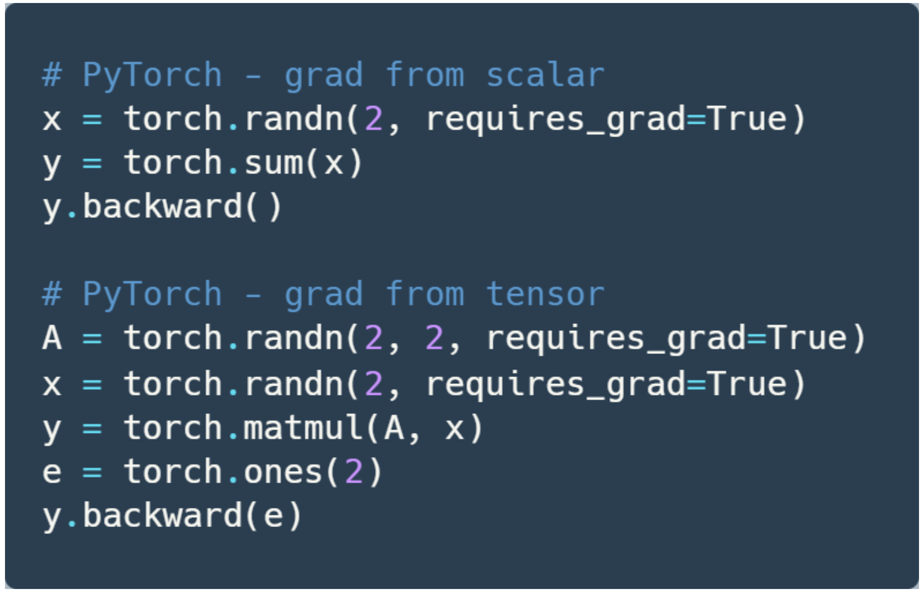

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y = torch.matmul(A, x)
e = torch.ones(2)
y.backward(e)
```

Backprop w/ layer-wise AD

1. Recompute input (inverse layer)
2. Forward pass w/ tracking enabled
3. Call torch autograd for layer
4. Extract + set gradients
5. Return original input + grads

(**MemCNN**, **i-RIM**)[1-2]

---

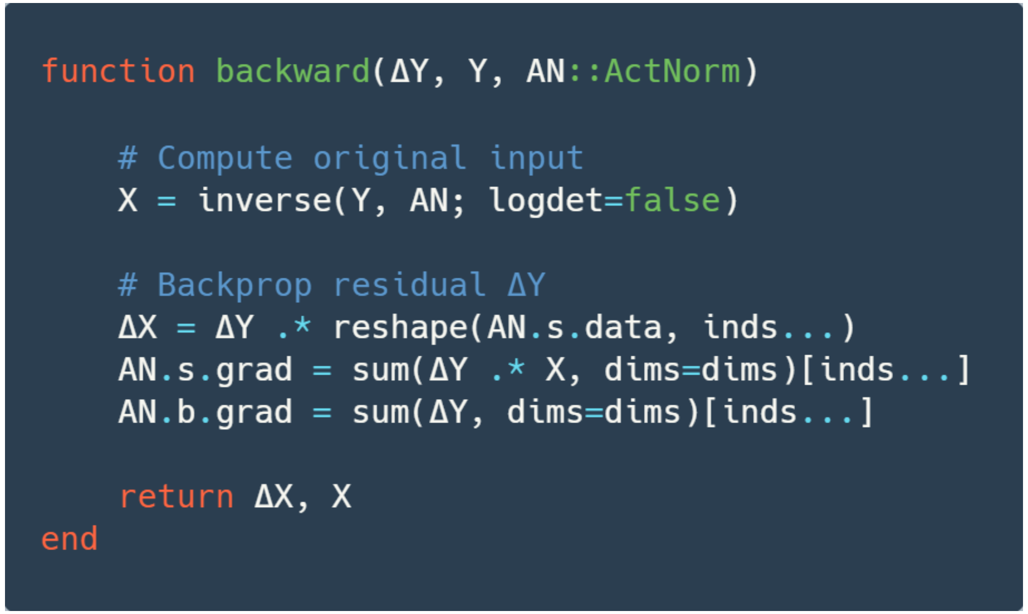
[1] Van de Leemput et al. *MemCNN: A Python/PyTorch package for creating memory-efficient INNs*, Journal of Open Source Software, 2019

[2] Putzky et al. *i-RIM applied to the fastMRI challenge*. ariXiv preprints, 2019.

Gradients & Jacobians

InvertibleNetworks

- All-at-once layer for inverse + backward pass
- No tracking of variables

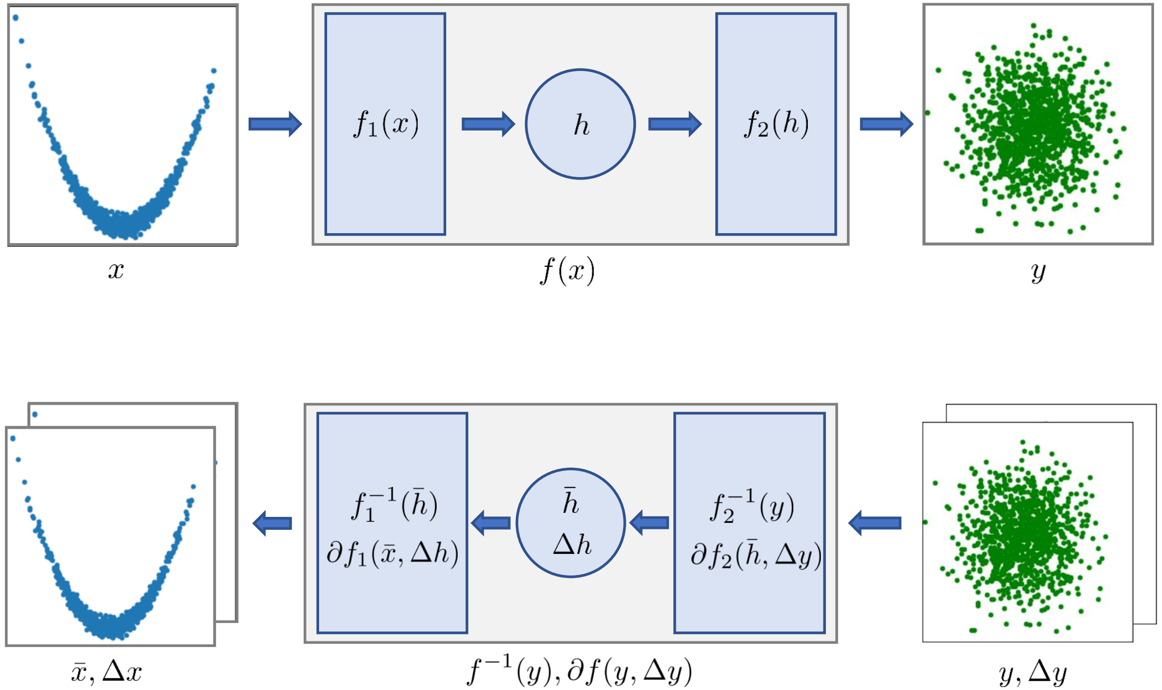


```
function backward(ΔY, Y, AN::ActNorm)

    # Compute original input
    X = inverse(Y, AN; logdet=false)

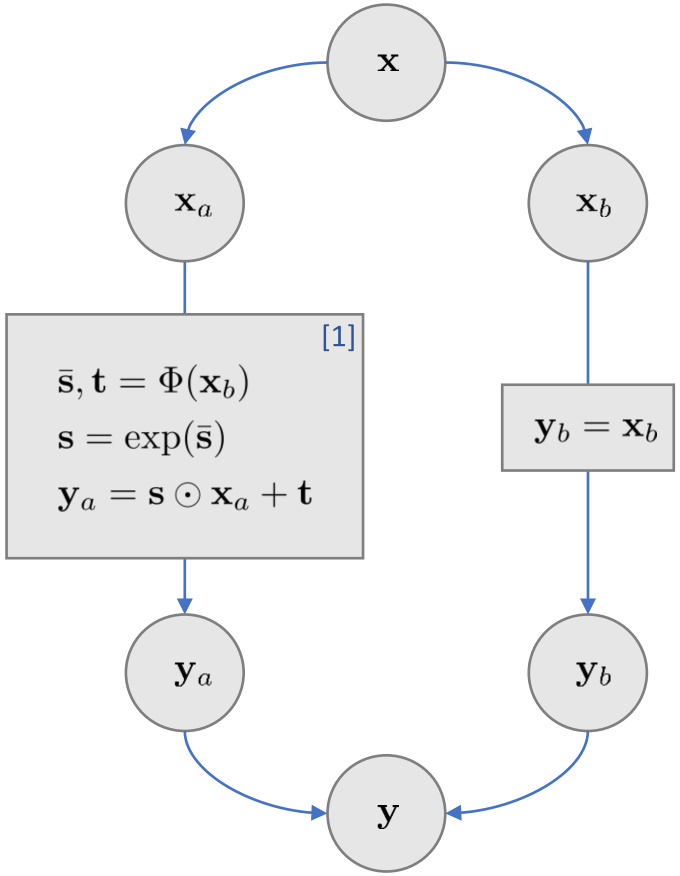
    # Backprop residual ΔY
    ΔX = ΔY .* reshape(AN.s.data, inds...)
    AN.s.grad = sum(ΔY .* X, dims=dims)[inds...]
    AN.b.grad = sum(ΔY, dims=dims)[inds...]

    return ΔX, X
end
```

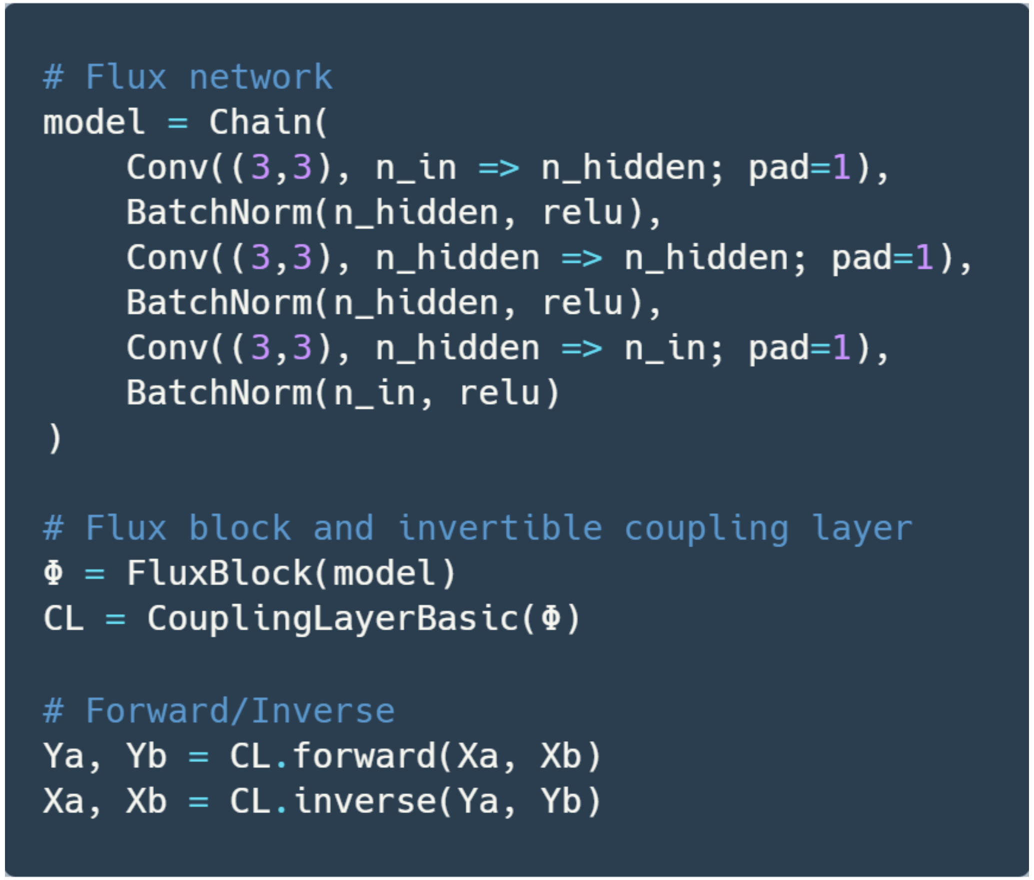


Integration with Flux.jl

Invertible coupling layers with Flux.jl



$\Phi(\mathbf{x})$: Shallow CNN/Res-Net



```
# Flux network
model = Chain(
    Conv((3,3), n_in => n_hidden; pad=1),
    BatchNorm(n_hidden, relu),
    Conv((3,3), n_hidden => n_hidden; pad=1),
    BatchNorm(n_hidden, relu),
    Conv((3,3), n_hidden => n_in; pad=1),
    BatchNorm(n_in, relu)
)

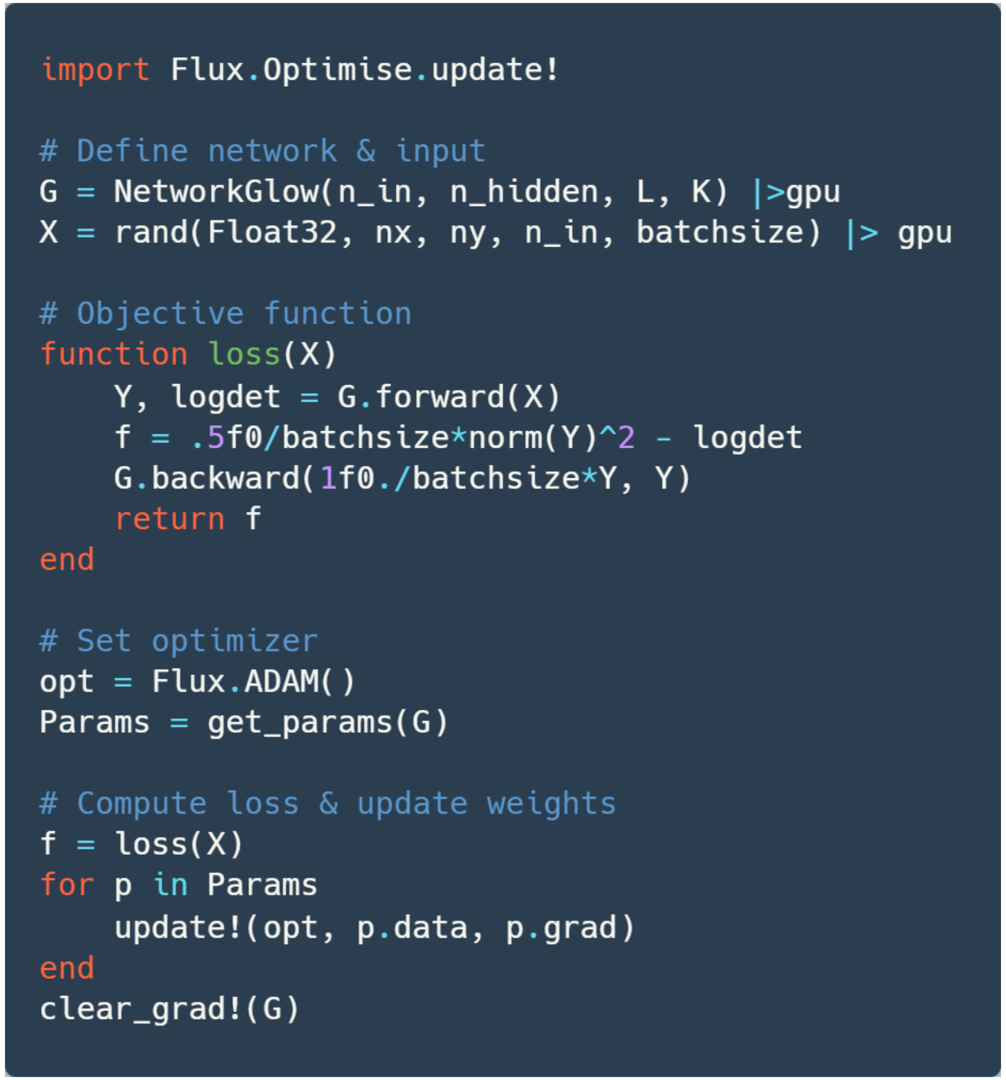
# Flux block and invertible coupling layer
Φ = FluxBlock(model)
CL = CouplingLayerBasic(Φ)

# Forward/Inverse
Ya, Yb = CL.forward(Xa, Xb)
Xa, Xb = CL.inverse(Ya, Yb)
```

[1] Dinh et al., *Nice: Non-linear independent component estimation*. arXiv preprints, 2014.

[1] Innes et al., Flux.jl, https://github.com/FluxML/Flux.jl, 2021

Integration with Flux.jl



```
import Flux.Optimise.update!

# Define network & input
G = NetworkGlow(n_in, n_hidden, L, K) |>gpu
X = rand(Float32, nx, ny, n_in, batchsize) |> gpu

# Objective function
function loss(X)
    Y, logdet = G.forward(X)
    f = .5f0/batchsize*norm(Y)^2 - logdet
    G.backward(1f0./batchsize*Y, Y)
    return f
end

# Set optimizer
opt = Flux.ADAM()
Params = get_params(G)

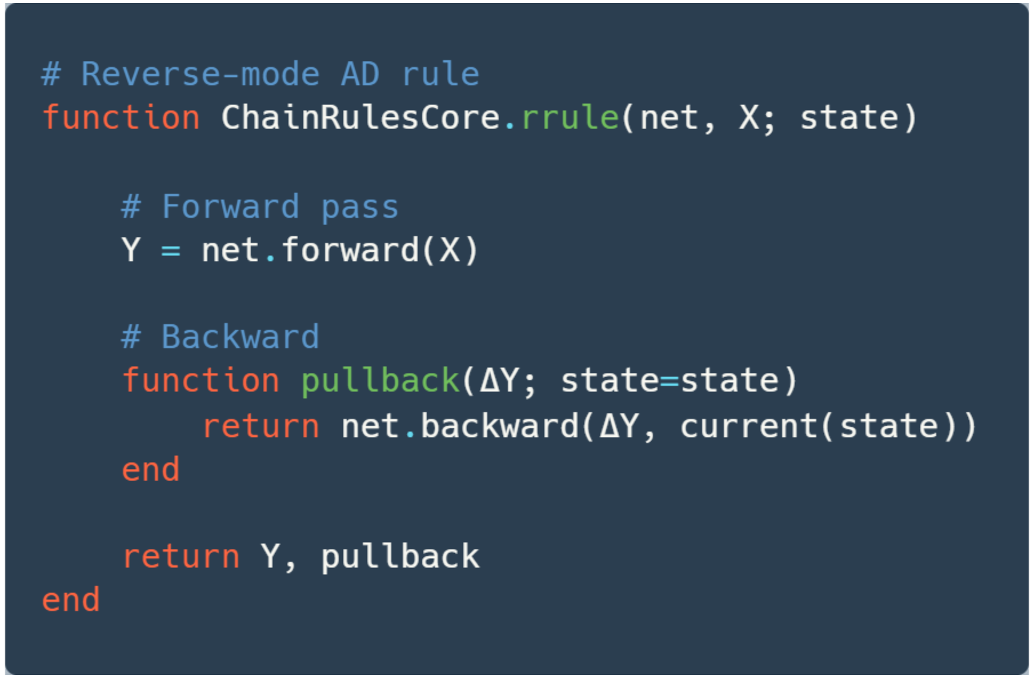
# Compute loss & update weights
f = loss(X)
for p in Params
    update!(opt, p.data, p.grad)
end
clear_grad!(G)
```

- Training INNs with Flux [1]
    - Flux optimizers (ADAM, etc.)
    - Update weights of INNs
    - Same as Flux networks

[1] Innes et al., *Flux.jl*, https://github.com/FluxML/Flux.jl, 2021
[2] White et al., *JuliaDiff/ChainRules.jl*, https://github.com/JuliaDiff/ChainRules.jl, 2021

Integration with ChainRules.jl

- Combine INN & Flux layers via ChainRules.jl [1-2]



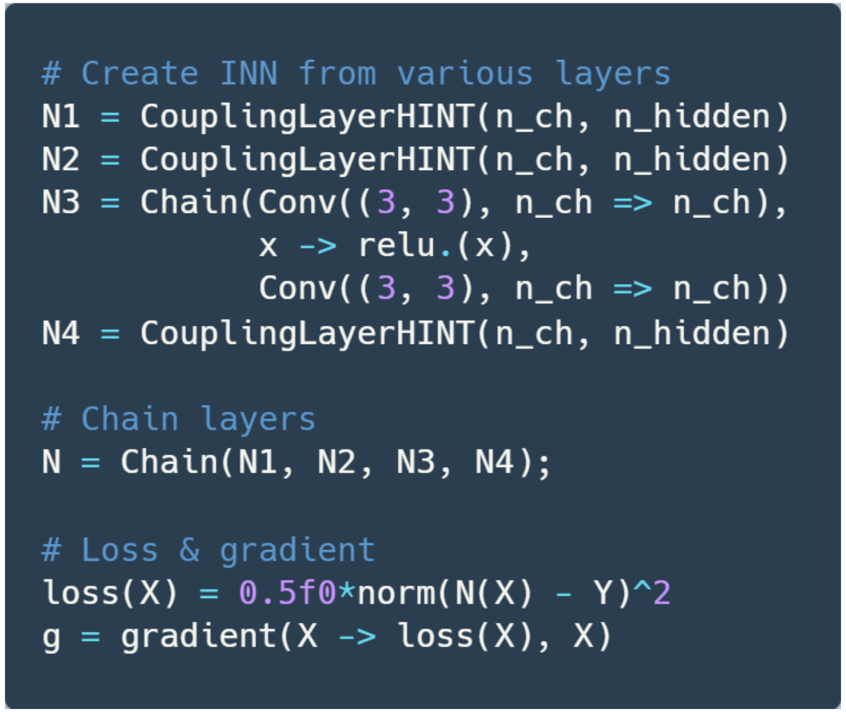
```
# Reverse-mode AD rule
function ChainRulesCore.rrule(net, X; state)

    # Forward pass
    Y = net.forward(X)

    # Backward
    function pullback(ΔY; state=state)
        return net.backward(ΔY, current(state))
    end

    return Y, pullback
end
```

ChainRule definition for reverse differentiation



```
# Create INN from various layers
N1 = CouplingLayerHINT(n_ch, n_hidden)
N2 = CouplingLayerHINT(n_ch, n_hidden)
N3 = Chain(Conv((3, 3), n_ch => n_ch),
           x -> relu.(x),
           Conv((3, 3), n_ch => n_ch))
N4 = CouplingLayerHINT(n_ch, n_hidden)

# Chain layers
N = Chain(N1, N2, N3, N4);

# Loss & gradient
loss(X) = 0.5f0*norm(N(X) - Y)^2
g = gradient(X -> loss(X), X)
```

Define multi-layer INN

Unit tests

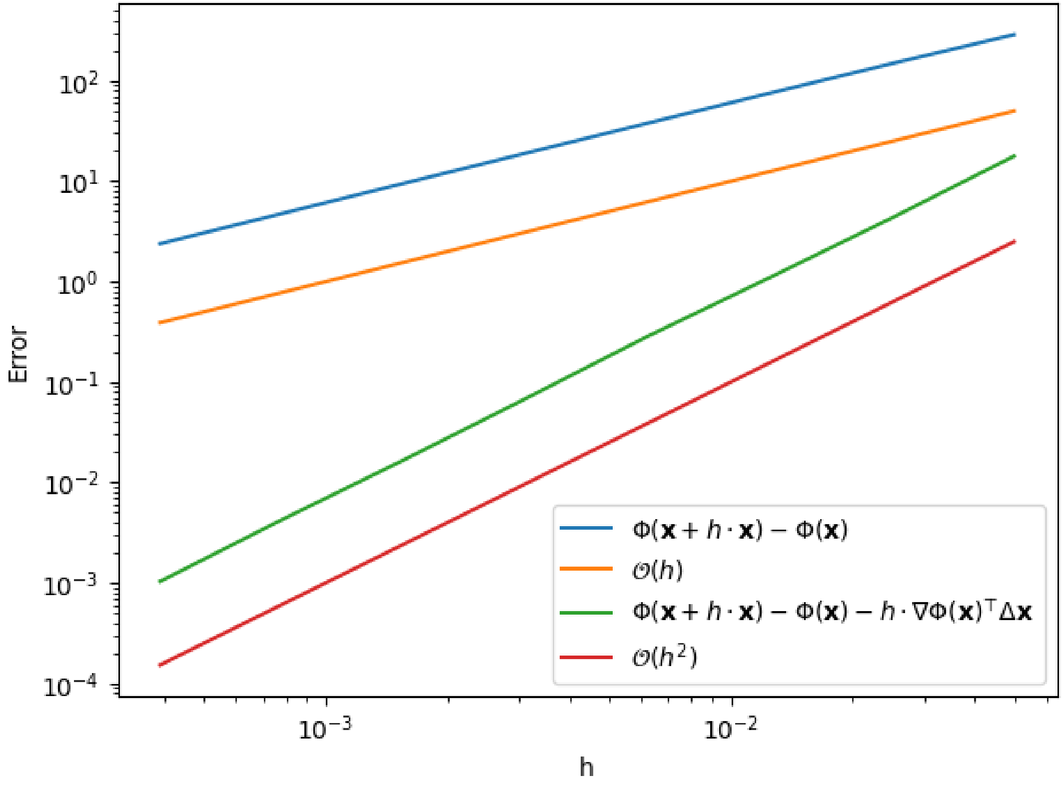
- Adjoint tests for linear operators:

$$\epsilon \leq \langle \mathbf{A}\mathbf{x}, \mathbf{y} \rangle - \langle \mathbf{A}^\top \mathbf{y}, \mathbf{x} \rangle$$

- Gradient tests for (non-) linear layers:

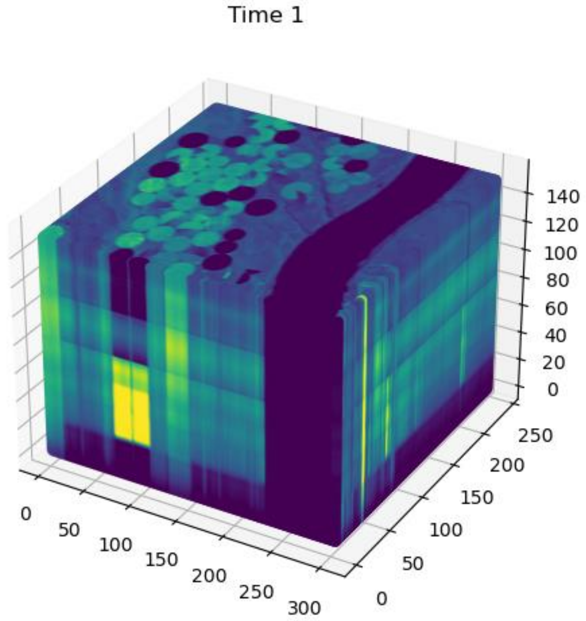
$$\Phi(\mathbf{x} + h \cdot \Delta\mathbf{x}) - \Phi(\mathbf{x}) = \mathcal{O}(h)$$
$$\Phi(\mathbf{x} + h \cdot \Delta\mathbf{x}) - \Phi(\mathbf{x}) - h \cdot \nabla\Phi(\mathbf{x})^\top \Delta\mathbf{x} = \mathcal{O}(h^2)$$

$$\Phi(\mathbf{w} + h \cdot \Delta\mathbf{w}) - \Phi(\mathbf{w}) = \mathcal{O}(h)$$
$$\Phi(\mathbf{w} + h \cdot \Delta\mathbf{w}) - \Phi(\mathbf{w}) - h \cdot \nabla\Phi(\mathbf{w})^\top \Delta\mathbf{w} = \mathcal{O}(h^2)$$



Gradient test for Glow network

Examples & applications



- Example applications
  - Inverse problems & loop unrolling
  - Image segmentation with partial labels and/or weak supervision
  - Normalizing flows & Bayesian inference

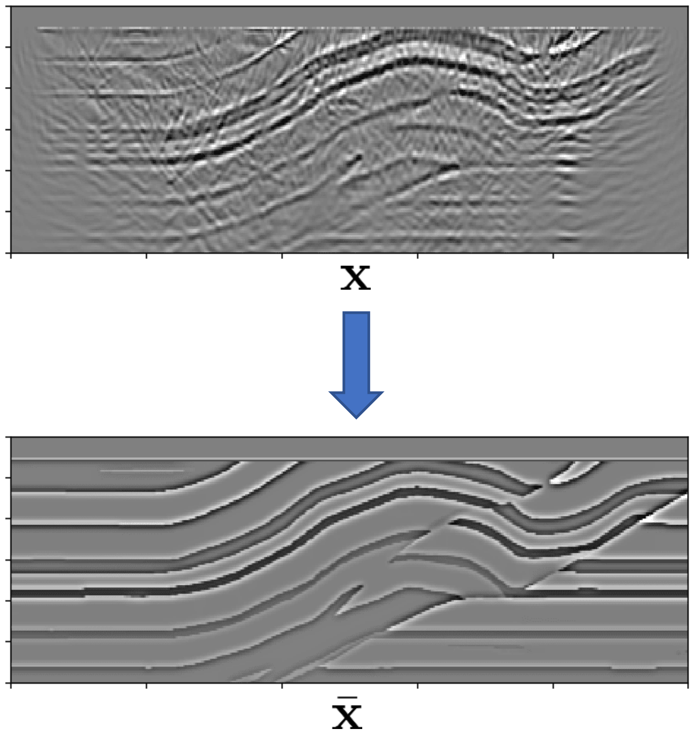
- All examples implemented with InvertibleNetworks.jl
  - Reproducible examples at https://github.com/slimgroup/InvertibleNetworks.jl/tree/master/examples

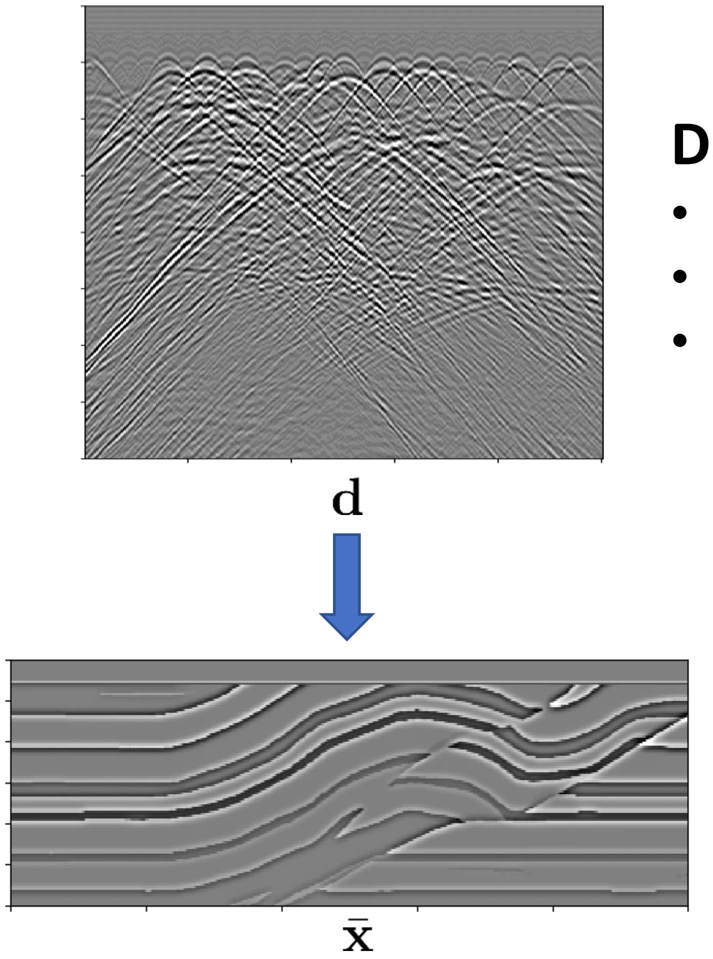
e.g. [1] Adler & Öktem., *Solving ill-posed inverse problems using iterative deep neural networks.jl,* Inverse Problems, 33, 2017
[2] Jin et al. *Deep convolutional neural network for inverse problems in imaging*. IEEE Transactions on Image Processing, 26 (9), 2017

Scenario 1: Loop-unrolled inverse problems [1-2]

Image-to-image mapping

- Learned denoiser/all-at-once
- Fully data-driven





Data-to-image mapping

- Data $\mathbf{d} = \mathbf{J}\mathbf{x}$
- Fully data-driven *or*
- Physics-augmented/iterative (use operator $\mathbf{J}$)

[1] Putzky & Welling, *Recurrent inference machines for solving inverse problems*, arXiv preprints, 2017
[2] Putzky & Welling, *Invert to learn to invert*, NIPS Proceedings, 2019

Scenario 1: Loop-unrolled inverse problems

Objective function for supervised learning

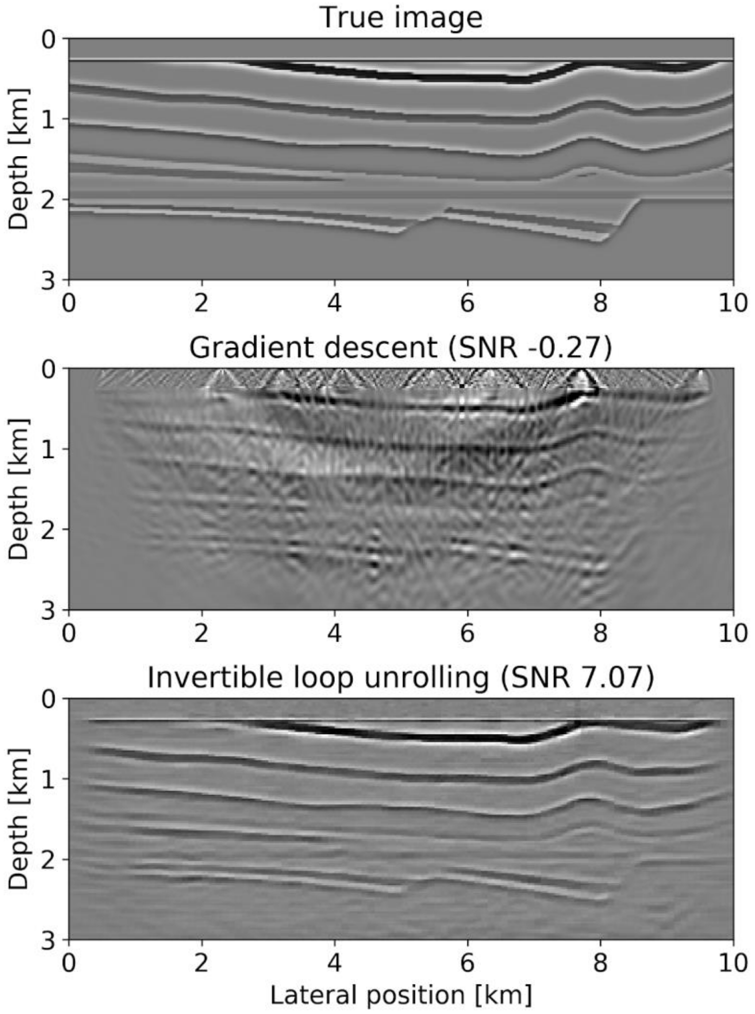
$$\underset{\theta}{\text{minimize}} \sum_{i=1}^{n_{\text{train}}} \frac{1}{2}\|\mathcal{G}_\theta(\mathbf{J}_i, \mathbf{d}_i) - \bar{\mathbf{x}}_i\|_2^2$$

with

```
function $\mathcal{G}(\mathbf{J}, \mathbf{d})$
    $\mathbf{x} = 0$
    for $j = 1, ..., n$
        $\mathbf{x} = \mathbf{Q}\mathbf{x}$
        $\mathbf{x}'_1 = \mathbf{x}_1$
        $\mathbf{g} = \mathbf{J}^\top(\mathbf{J}\mathbf{x}'_1[1] - \mathbf{d})$
        $\mathbf{s}', \mathbf{t} = \mathrm{NN}([\mathbf{g}, \mathbf{x}'_1[2{:}\mathrm{end}]])$
        $\mathbf{s} = \sigma(\mathbf{s}')$
        $\mathbf{x}'_2 = \mathbf{x}_2 \odot \mathbf{s} + \mathbf{t}$
        $\mathbf{x} = \mathbf{Q}^\top\mathbf{x}'$
    end
    return $\mathbf{x}$
end
```

Invertible recurrent inference machine (i-RIM)[1-2]

Results after
4 training epochs



[1] Putzky & Welling, *Recurrent inference machines for solving inverse problems*, arXiv preprints, 2017
[2] Putzky & Welling, *Invert to learn to invert*, NIPS Proceedings, 2019

Scenario 1: Loop-unrolled inverse problems

Objective function for supervised learning

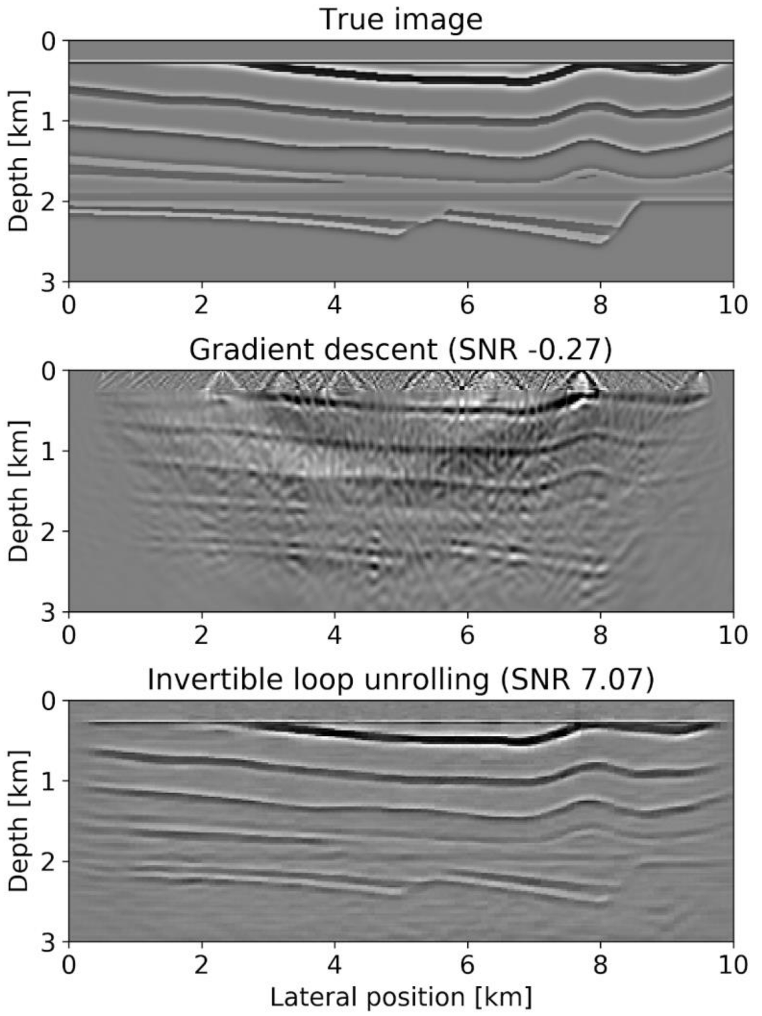
$$\underset{\theta}{\text{minimize}} \sum_{i=1}^{n_{\text{train}}} \frac{1}{2}\|\mathcal{G}_\theta(\mathbf{J}_i,\mathbf{d}_i)-\bar{\mathbf{x}}_i\|_2^2$$

with

```
function $\mathcal{G}(\mathbf{J},\mathbf{d})$
    $\mathbf{x}=0$
    for $j=1,...,n$
        $\mathbf{x}=\mathbf{Q}\mathbf{x}$
        $\mathbf{x}_1'=\mathbf{x}_1$
        $\mathbf{g}=\mathbf{J}^\top(\mathbf{J}\mathbf{x}_1'[1]-\mathbf{d})$
        $\mathbf{s}',\mathbf{t}=\mathrm{NN}([\mathbf{g},\mathbf{x}_1'[2\text{:end}]])$
        $\mathbf{s}=\sigma(\mathbf{s}')$
        $\mathbf{x}_2'=\mathbf{x}_2\odot\mathbf{s}+\mathbf{t}$
        $\mathbf{x}=\mathbf{Q}^\top\mathbf{x}'$
    end
    return $\mathbf{x}$
end
```

Invertible recurrent inference machine (i-RIM)[1-2]

Results after 4 training epochs


True image

Gradient descent (SNR -0.27)

Invertible loop unrolling (SNR 7.07)

Scenario 1: Loop-unrolled inverse problems

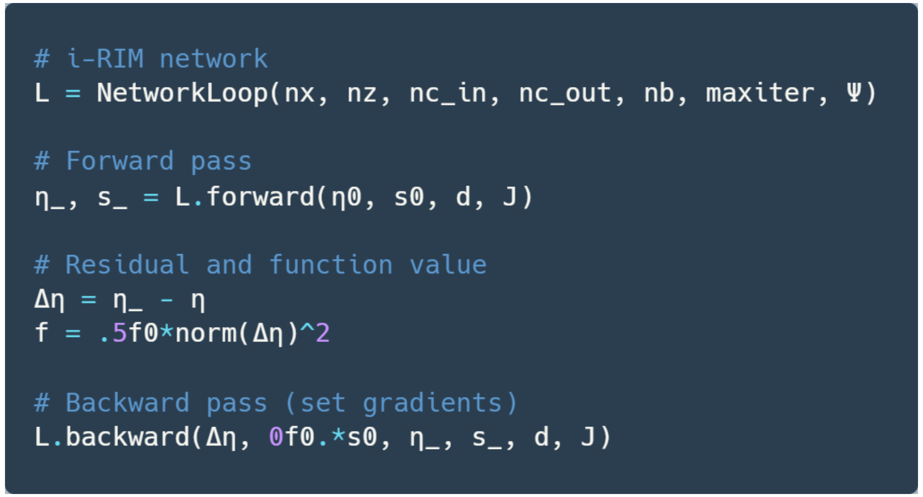
Objective function for supervised learning

$$\underset{\theta}{\text{minimize}} \sum_{i=1}^{n_{\text{train}}} \frac{1}{2} \|\mathcal{G}_\theta(\mathbf{J}_i, \mathbf{d}_i) - \bar{\mathbf{x}}_i\|_2^2$$

with

```
function $\mathcal{G}(\mathbf{J}, \mathbf{d})$
    $\mathbf{x} = 0$
    for $j = 1, ..., n$
        $\mathbf{x} = \mathbf{Q}\mathbf{x}$
        $\mathbf{x}_1' = \mathbf{x}_1$
        $\mathbf{g} = \mathbf{J}^\top(\mathbf{J}\mathbf{x}_1'[1] - \mathbf{d})$
        $\mathbf{s}', \mathbf{t} = \mathrm{NN}([\mathbf{g}, \mathbf{x}_1'[2{:}\mathrm{end}]])$
        $\mathbf{s} = \sigma(\mathbf{s}')$
        $\mathbf{x}_2' = \mathbf{x}_2 \odot \mathbf{s} + \mathbf{t}$
        $\mathbf{x} = \mathbf{Q}^\top \mathbf{x}'$
    end
    return $\mathbf{x}$
end
```

Implementation



```
# i-RIM network
L = NetworkLoop(nx, nz, nc_in, nc_out, nb, maxiter, Ψ)

# Forward pass
η_, s_ = L.forward(η0, s0, d, J)

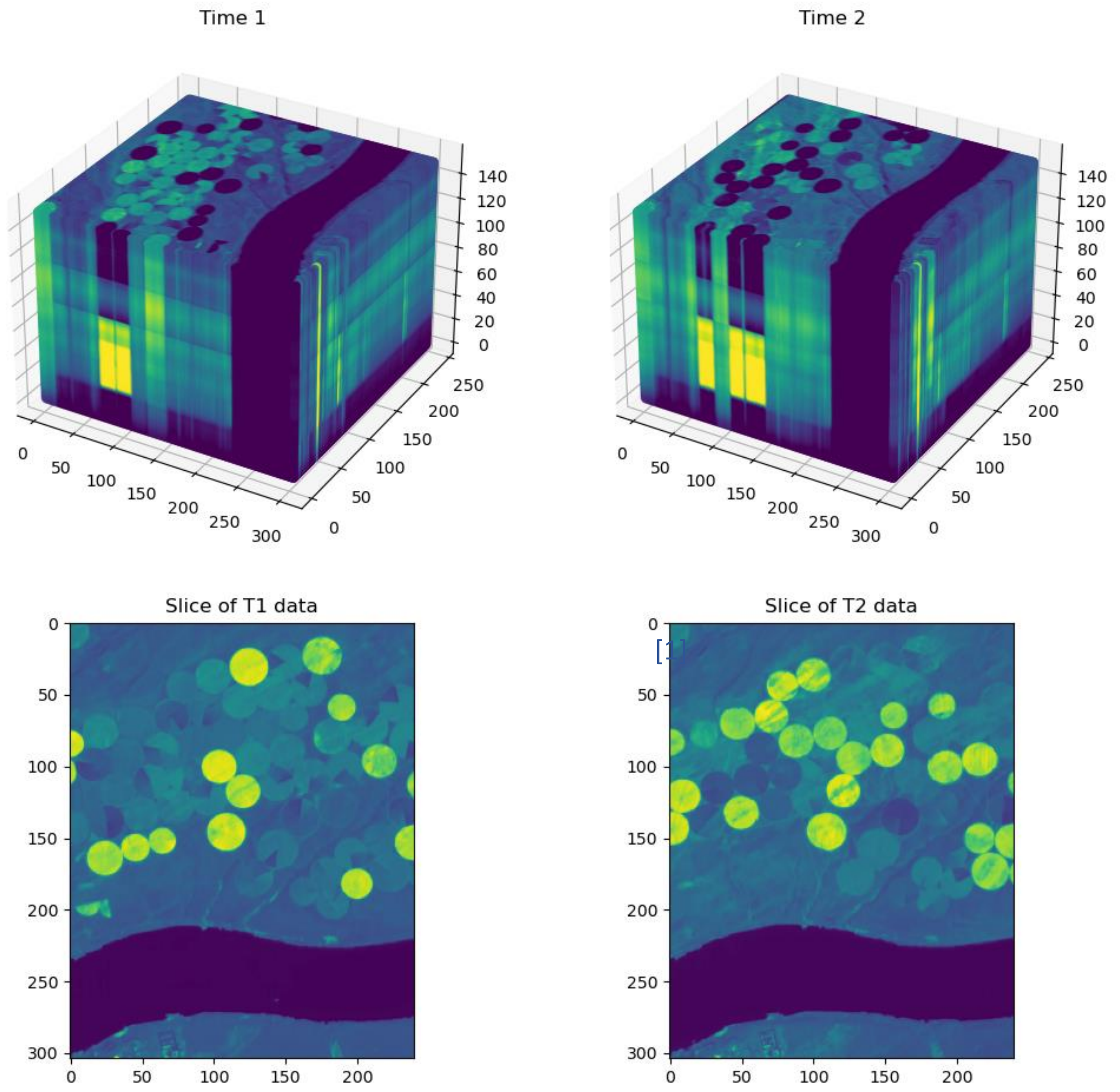
# Residual and function value
Δη = η_ - η
f = .5f0*norm(Δη)^2

# Backward pass (set gradients)
L.backward(Δη, 0f0.*s0, η_, s_, d, J)
```

Compatible w/ matrix-free linear operators

Scenario 2: 4D image segmentation

- Time-lapse hyper-spectral land use change [1]
  - Single large-scale 4D input volume (307 x 241 x 154 x 2)
  - 18 layer invertible hyperbolic net with 3D convolutions
  - Coupled space-frequency approach
  - 128 channels



Time 1

Time 2

Slice of T1 data

Slice of T2 data

---

[1] Peters et al., Fully reversible neural networks for large-scale surface and sub-surface characterization via remote sensing. arXiv preprints, 2020.

Scenario 2: 4D image segmentation

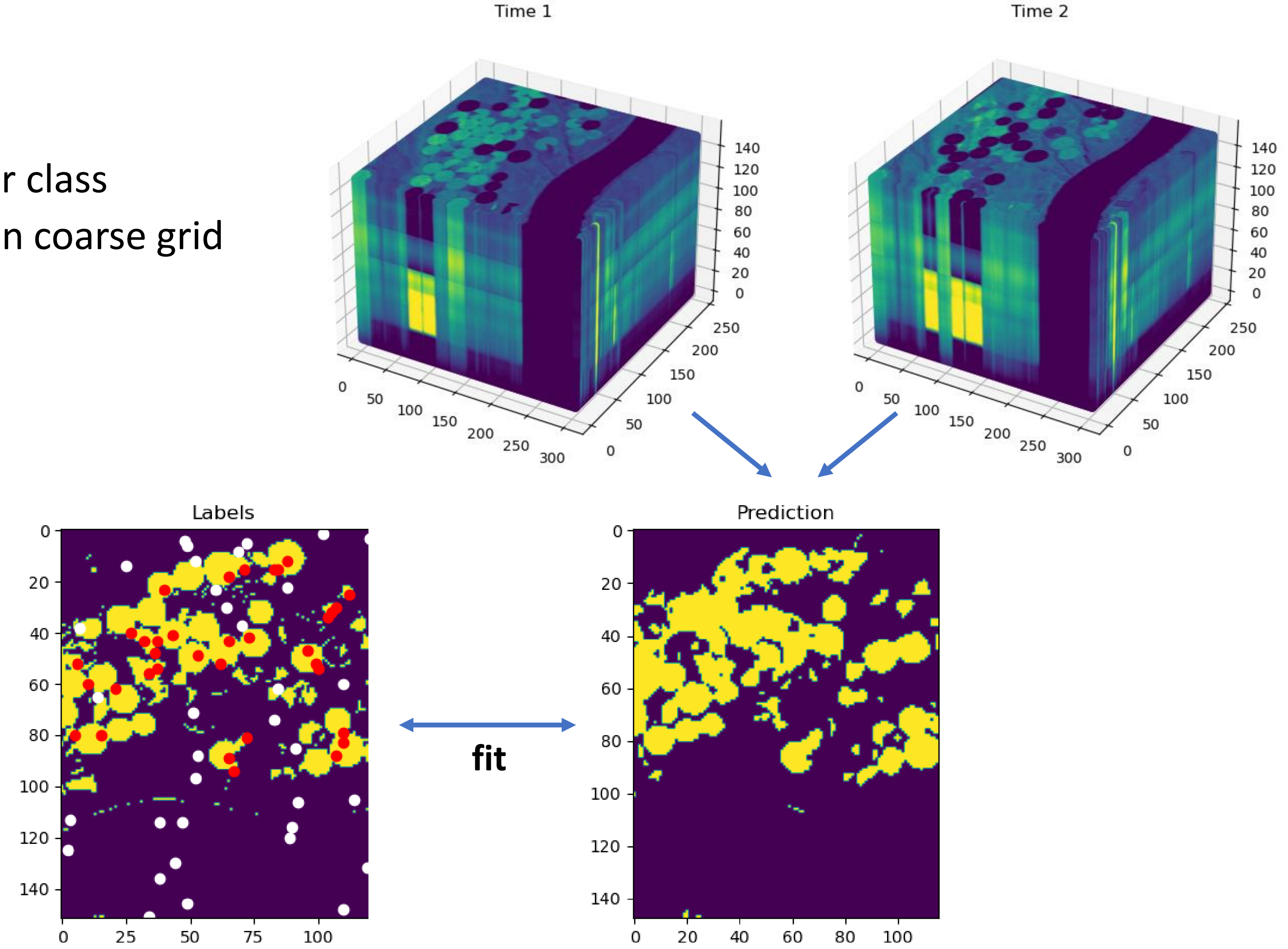
Goal: predict land use change

- Only 35 point annotations per class
- Predict change everywhere on coarse grid

Memory requirements

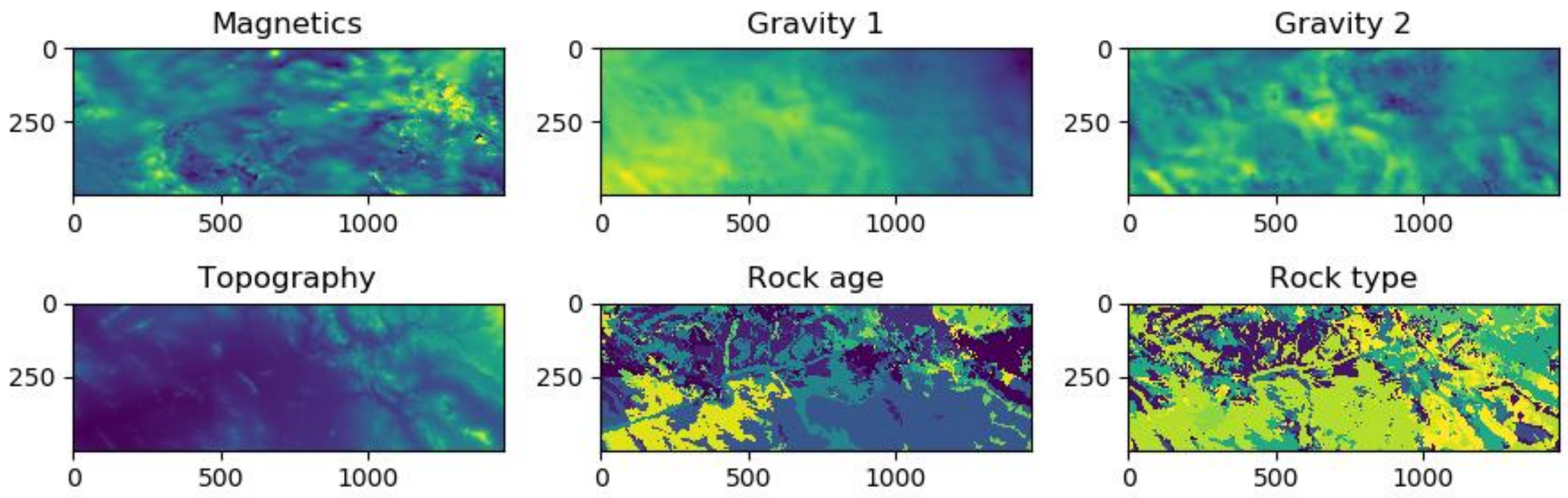
- 18 layer INN, 128 channels
- Image: 307 x 241 x 154 x 2
- Invertible hyperbolic net: **17 GB**
- Non-invertible equivalent: **307 GB**

Enable deeper networks and/or larger data sets

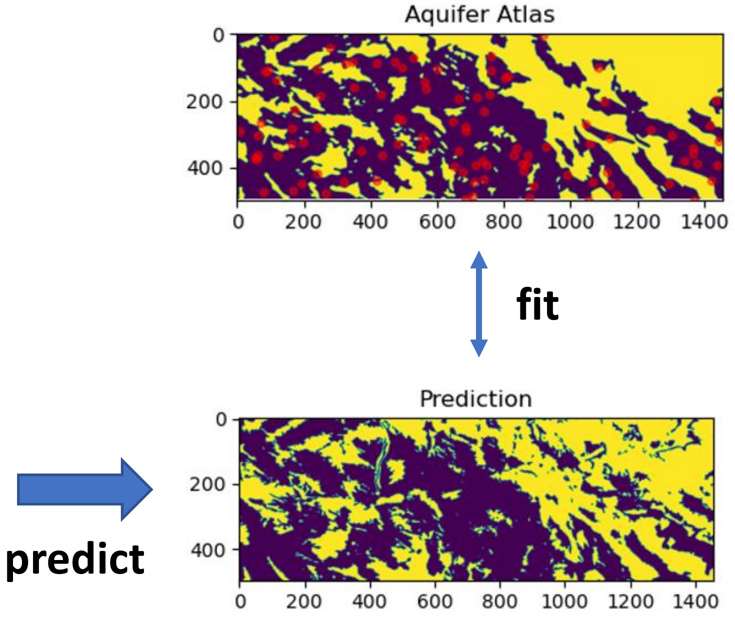


Scenario 3: Weakly supervised segmentation

- Goal: Map out geological aquifers from multi-modal geophysical data [1]
  - Class 1: partial point annotations
  - Class 2: No labels, occupies ~50 to 65 % per domain
  - Learn from partial label + priors using *constrained optimization*



Input data: 1,450 x 450 x 56

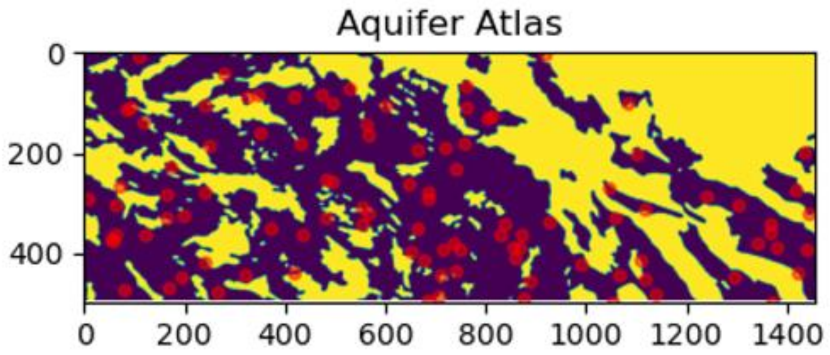


[1] Peters, Bas. Point-to-set distance functions for weakly supervised segmentation. arXiv preprints, 2021.

[1] Peters, Bas. Point-to-set distance functions for weakly supervised segmentation. arXiv preprints, 2021.

Scenario 3: Weakly supervised segmentation

- Translate partial labels + prior information
  → convex constraints



- Constraints on network output $\mathbf{y} = g(\mathbf{K}, \mathbf{d})$ (not on weights)

$\mathbf{K}$: Network weights
$\mathbf{d}$: Input data
$\mathbf{y}$: Output label

- Training: non-convex feasibility problem

$$\text{find}\, g(\mathbf{K}, \mathbf{d}) \in D \Leftrightarrow \min_{\mathbf{K}} \iota_D(g(\mathbf{K}, \mathbf{d}))$$

- Solve via projection-based point-to-set distance functions

$$d_D^2(\mathbf{y}) = \frac{1}{2}\|P_D(\mathbf{y}) - \mathbf{y}\|_2^2 \qquad \nabla_{\mathbf{y}} d_D^2(\mathbf{y}) = \mathbf{y} - P_D(\mathbf{y})$$

[1] Peters, Bas. Point-to-set distance functions for weakly supervised segmentation. arXiv preprints, 2021.

Scenario 3: Weakly supervised segmentation

- Train neural network as:

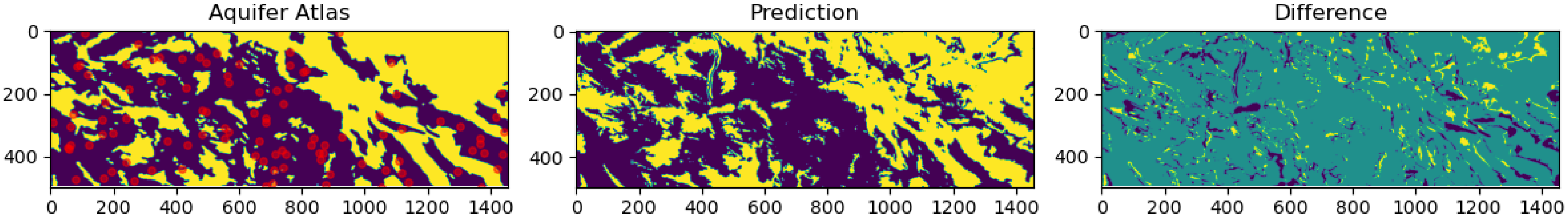
$$\min_{\mathbf{K}} \frac{1}{2}\|P_D(g(\mathbf{K},\mathbf{d})) - g(\mathbf{K},\mathbf{d})\|_2^2$$

Add INN as constraint

$$\xrightarrow{\hspace{4em}}$$

$$\begin{aligned}
&\min_{\{\mathbf{K}\}} \frac{1}{2}\|P_D(\mathbf{y}_n) - \mathbf{y}_n\|_2^2 \text{ s.t.}\\
&\mathbf{y}_n = \mathbf{y}_{n-1} - \sigma(\mathbf{K}_n\mathbf{y}_{n-1})\\
&\vdots\\
&\mathbf{y}_j = \mathbf{y}_{j-1} - \sigma(\mathbf{K}_j\mathbf{y}_{j-1})\\
&\vdots\\
&\mathbf{y}_1 = \mathbf{d},
\end{aligned}$$

- Form Lagrangian + conventional backpropagation
- Difference to previous examples using labels
  - Gradient of loss ⇨ gradient of distance function



Scenario 4: Normalizing flows & inference

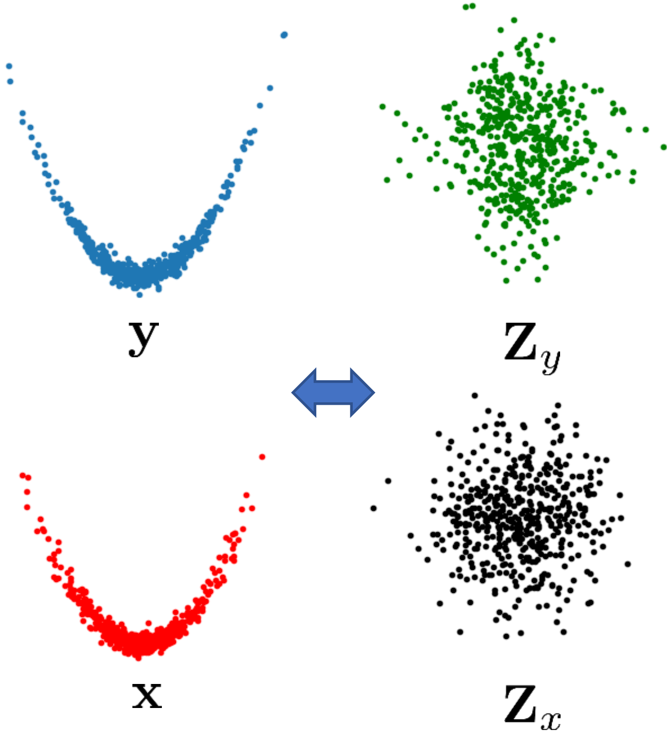
- Goal: perform Bayesian inference for data & image reconstruction [1-3]
- Train conditional INN $G_\theta : \mathcal{Y} \times \mathcal{X} \to \mathcal{Z}_y \times \mathcal{Z}_x$

$$\min_\theta \mathbb{E}_{\mathbf{y},\mathbf{x}\sim p(\mathbf{y},\mathbf{x})}\left[\frac{1}{2}\left\|G_\theta(\mathbf{y},\mathbf{x})\right\|^2 - \log\left|\det \nabla_{y,x}\, G_\theta(\mathbf{y},\mathbf{x})\right|\right]$$

$$G_\theta(\mathbf{y},\mathbf{x}) = \begin{bmatrix} G_{\theta_y}(\mathbf{y}) \\ G_{\theta_x}(\mathbf{y},\mathbf{x}) \end{bmatrix}, \quad \boldsymbol{\theta} = \begin{bmatrix} \boldsymbol{\theta}_y \\ \boldsymbol{\theta}_x \end{bmatrix}$$

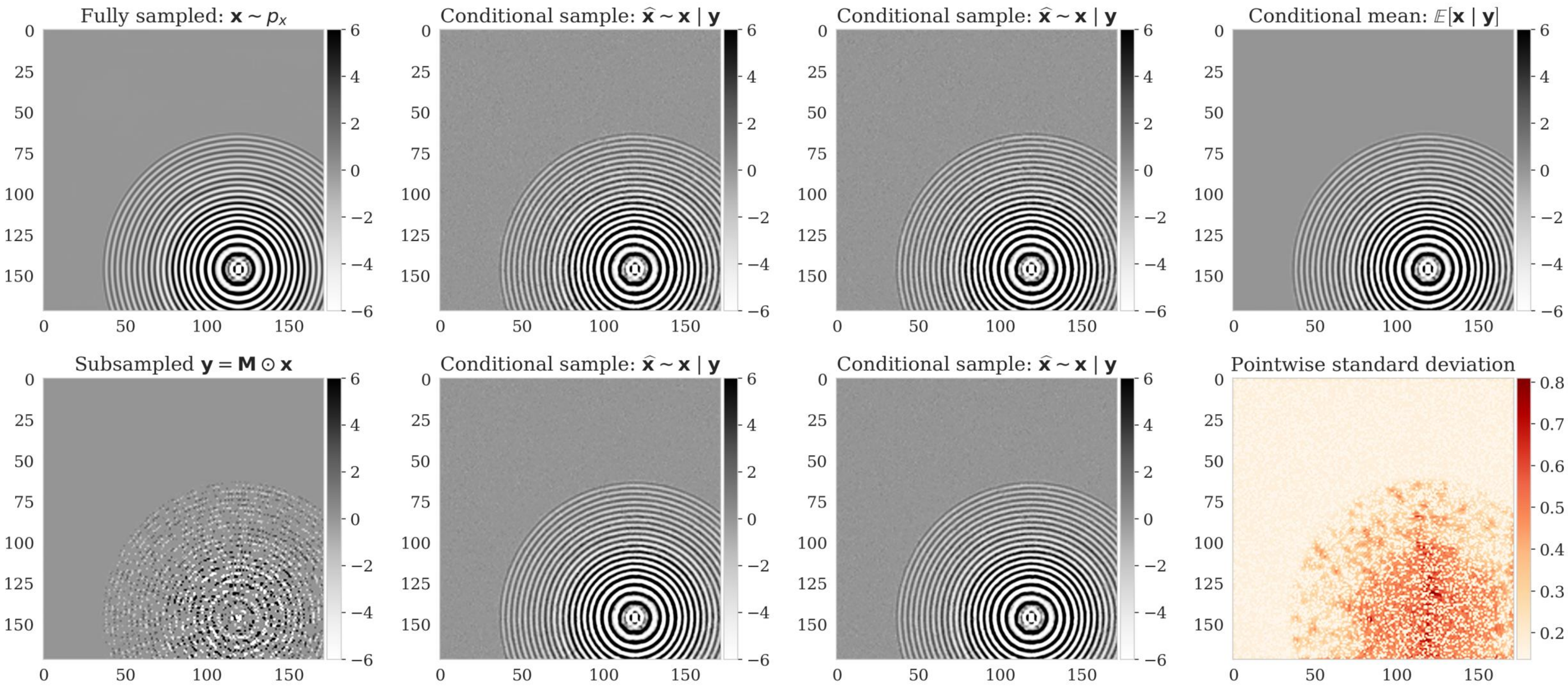
- Perform conditional sampling via

$$G_{\theta_x}^{-1}(G_{\theta_y}(\mathbf{y}),\mathbf{z}) \sim p(\mathbf{x} \mid \mathbf{y}), \quad \mathbf{z} \sim \mathrm{N}(\mathbf{0},\mathbf{I})$$



[1] Kruse et al., *HINT: Hierarchical Invertible Neural Transport for Density Estimation and Bayesian Inference*. Proceedings of AAAI, 2021
[2] Siahkoohi et al., *Preconditioned training of normalizing flows for variational inference for inverse problems*. 3rd Symposium on Advances in Approximate Bayesian Inference. 2021
[3] Rizzuti et al., Parameterizing uncertainty by deep invertible networks, an application to reservoir characterization. SEG, 2020.

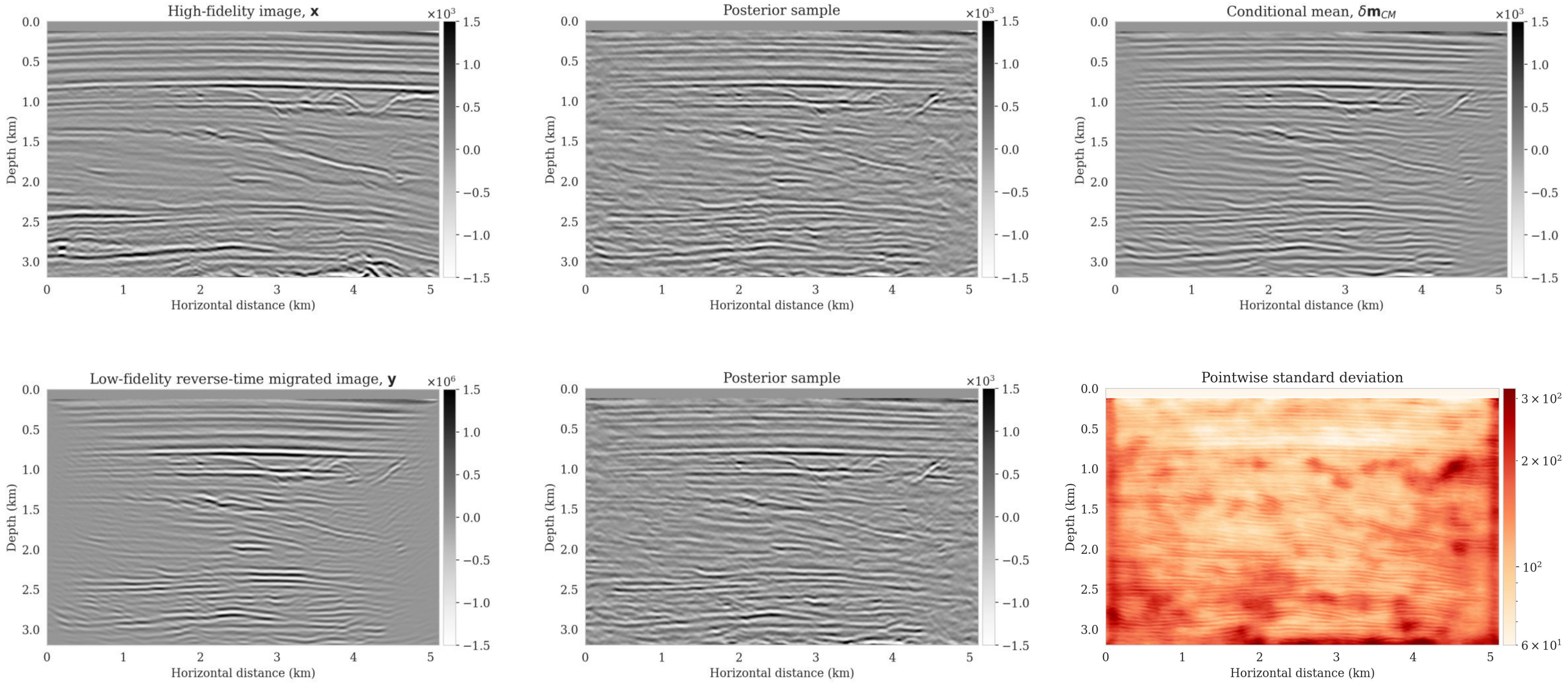
Scenario 4: Normalizing flows & inference



Seismic wavefield reconstruction

[1] Kumar et al., "Enabling uncertainty quantification for seismic data pre-processing using normalizing flows (NF) – an interpolation example. SEG, 2021

Scenario 4: Normalizing flows & inference

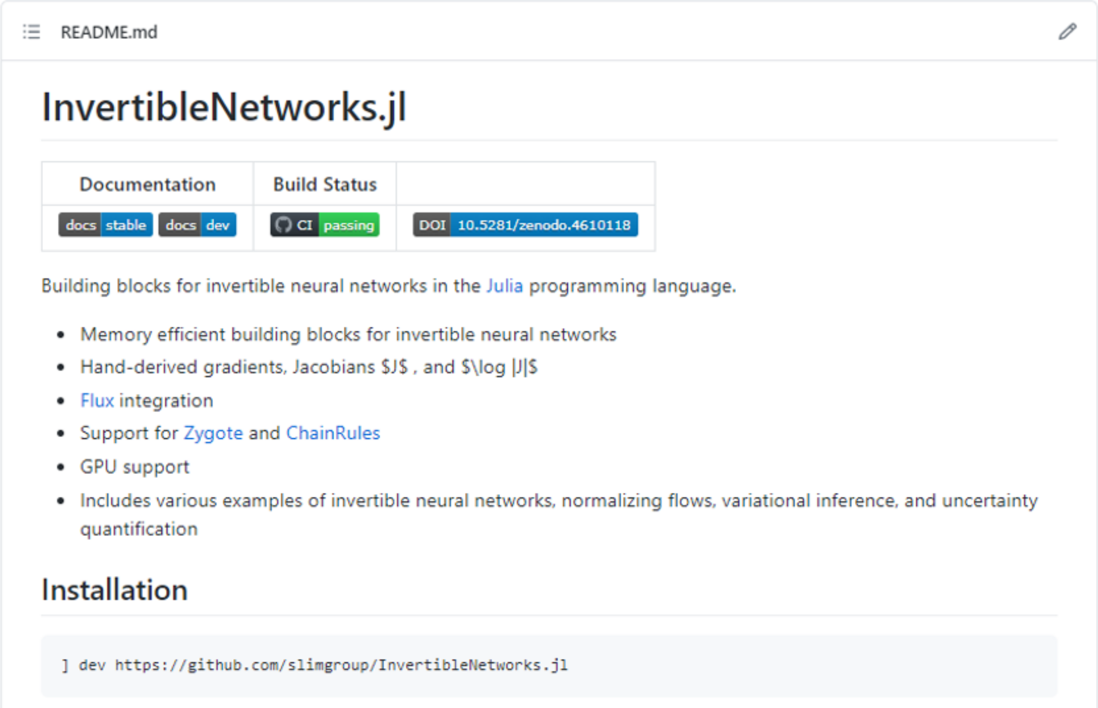


Seismic image reconstruction

[1] Siakhooi et al., Learning by example: fast reliability-aware seismic imaging with normalizing flows. SEG, 2021.

Summary & conclusions

- Invertible CNNs & Normalizing Flows in Julia language
- Memory efficient/optimal training
  - *Stateless* training
  - No extra forward evaluations
- Integration with Julia ecosystem
  - Flux.jl, ChainRules.jl, Zygote.jl
- Julia enables ML innovation
  - No comparable frameworks with PyTorch, TensorFlow, etc.



InvertibleNetworks.jl

Documentation	Build Status	
docs stable docs dev	CI passing	DOI 10.5281/zenodo.4610118

Building blocks for invertible neural networks in the Julia programming language.

- Memory efficient building blocks for invertible neural networks
- Hand-derived gradients, Jacobians J , and $\log |J|$
- Flux integration
- Support for Zygote and ChainRules
- GPU support
- Includes various examples of invertible neural networks, normalizing flows, variational inference, and uncertainty quantification

Installation

```
] dev https://github.com/slimgroup/InvertibleNetworks.jl
```

https://github.com/slimgroup/InvertibleNetworks.jl

Thank you for your attention

&

Thanks to the Georgia Research Alliance
and partners of the ML4Seismic Consortium

Georgia Tech

Seismic Laboratory for Imaging and Modeling