Equivariant Neural Networks for Inverse Problems

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Joint work with:
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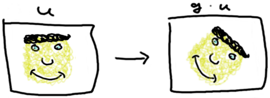
THE FARADAY INSTITUTION

Outline

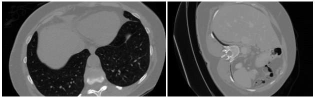
1) Inverse Problems
and Machine Learning

$$\min_x \frac{1}{2}\|Ax - y\|_2^2 + \lambda\mathcal{R}(x)$$

2) Equivariance
and Neural Networks



3) Numerical Results
for CT and MRI



Celledoni et al., Equivariant neural networks for inverse problems,
to appear in Inverse Problems, 2021

Inverse Problems and Machine Learning

Inverse problems

$$Au = b$$

u : desired solution

b : observed data

A : mathematical model

Goal: recover u given b

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- b : observed data
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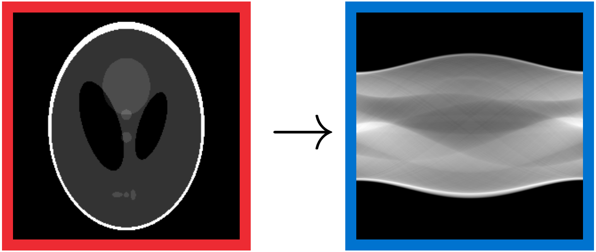
Goal: recover u given b

- Radon / X-ray transform (e.g. CT, PET) $Au(L) = \int_L u(x)dx$



Inverse problems

$$Au = b$$

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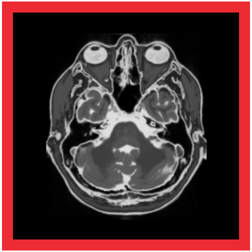
Goal: recover u given b

- Fourier transform (e.g. MRI) $Au(k) = \int u(x) \exp(-ikx) dx$



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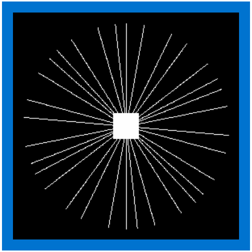
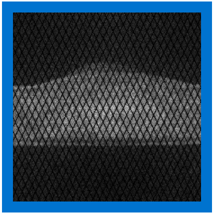
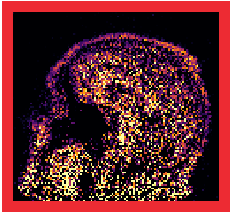


What is the problem with inverse problems?

- $Au(L) = \int_L u(x)dx$





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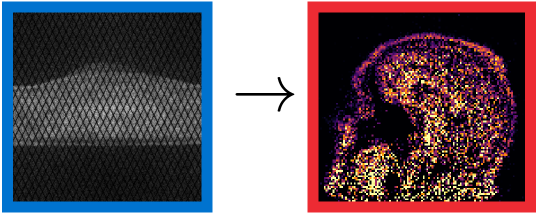

Hadamard (1902): We call an inverse problem $Au = b$ **well-posed** if

(1) a solution u^* **exists**

(2) the solution u^* is **unique**

(3) u^* depends **continuously** on data b.

Otherwise, it is called **ill-posed**.

Jacques Hadamard

Most interesting problems are **ill-posed**.

How to solve inverse problems?

Variational regularization

Approximate a solution u^* of $Au = b$ via

$$\hat{u} \in \arg\min_u \left\{ \mathcal{D}(u) + \lambda \mathcal{R}(u) \right\}$$

$\mathcal{D}$ measures **fidelity** between Au and b, related to noise statistics

$\mathcal{R}$ **regularizer** penalizes unwanted features and ensures stability

$\lambda \geq 0$ **regularization parameter** balances fidelity and regularization

Scherzer et al. 2008, Ito and Jin 2015, Benning and Burger 2018

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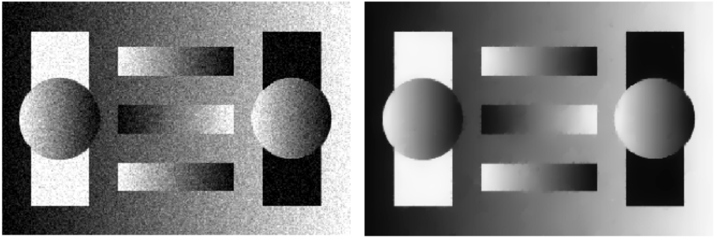
- squared L^2 norm: $\mathcal{R}(u) = \frac{1}{2}\|u\|_2^2$
- squared H^1 semi-norm: $\mathcal{R}(u) = \frac{1}{2}\|\nabla u\|_2^2$
- Total Variation $\mathcal{R}(u) = \|\nabla u\|_1$ Rudin, Osher, Fatemi 1992
- Total Generalized Variation
  $\mathcal{R}(u) = \inf_v \|\nabla u - v\|_1 + \beta\|\nabla v\|_1$ Bredies, Kunisch, Pock 2010



Noisy image TGV^2 denoised image

How to ACTUALLY solve inverse problems?

$$\hat{u} \in \arg\min_{u} \left\{ \mathcal{D}(u) + \lambda \mathcal{R}(u) \right\}$$

Forward-Backward Splitting Beck and Teboulle 2009

$$u^{k+1} = \text{prox}_{\tau^k \lambda \mathcal{R}}(u^k - \tau^k \nabla \mathcal{D}(u^k))$$

Solution $\Phi(b) := \lim_{k \to \infty} u^k$.
Choose τ^k, λ: $\Phi(b) = \hat{u} \to u^*$ if $\lambda \to 0$

Proximal operator Moreau 1962

$$\text{prox}_f(z) := \arg\min_u \frac{1}{2}\|u - z\|^2 + f(u)$$

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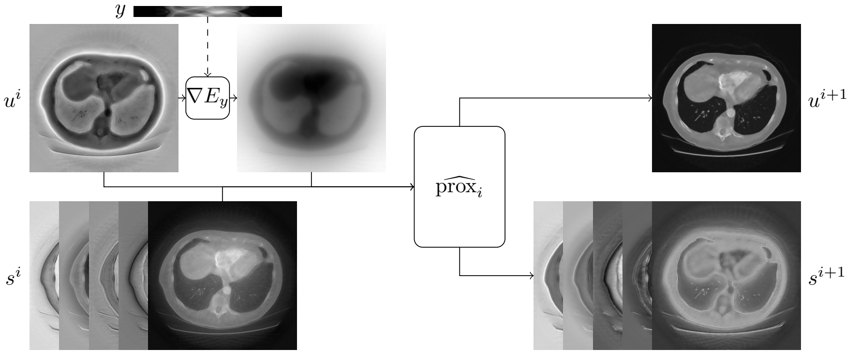
Learned gradient descent Adler and Öktem 2017

$$u^{k+1} = \widehat{\text{prox}_i}(u^k, \nabla \mathcal{D}(u^k))$$

Solution $\Phi(b) := u^K$, "small" $K \in \mathbb{N}$.
Learn $\widehat{\text{prox}_i}$: $\Phi(b) \approx u^*$

Learned proximal gradient descent with memory

- memory s



Equivariance and Neural Networks

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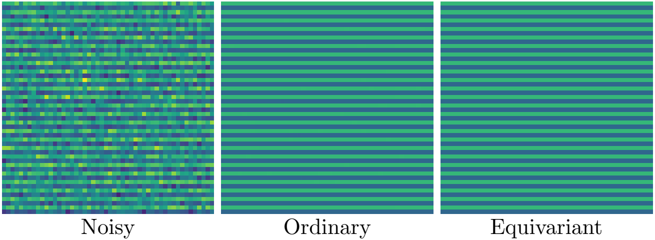

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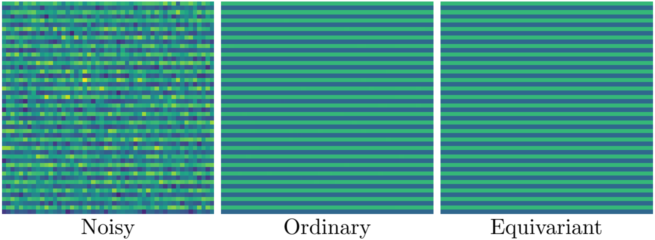

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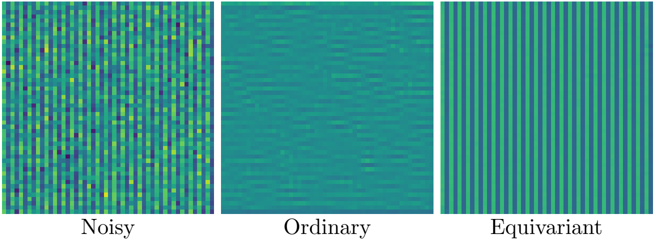

How to get "equivariant" mappings?

Example: R_θ rotation by θ, Φ denoising network

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- **data augmentation**: e.g. $(b_i, u_i)_i$ becomes $(R_\theta b_i, R_\theta u_i)_{i,\theta}$
  - ✓ **simple to implement** for image-based tasks (e.g. denoising, image segmentation etc)
  - ✗ potentially **computationally costly** since training data is larger
  - ✗ **no guarantees** this will translate to test data
  - ✗ **not always easy/possible** (for inverse problems only viable in simulations or if data is not paired (semi-supervised training))

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  - ✗ **no guarantees** this will translate to test data
  - ✗ **not always easy/possible** (for inverse problems only viable in simulations or if data is not paired (semi-supervised training))
- **equivariance by design** (this talk!)
  - ✓ **mathematical guarantees**
  - ✗ **not trivial** to do

Equivariant neural networks have been studied a lot for segmentation, classification, denoising etc Bekkers et al. 2018, Weiler and Cesa 2019, Cohen and Welling 2016, Dieleman et al. 2016, Sosnovik et al. 2019, Worall and Welling 2019, ...

What is equivariance?

Definition (Group G)

- **associativity:** $\forall g_1, g_2, g_3 \in G : (g_1 \cdot g_2) \cdot g_3 = g_1 \cdot (g_2 \cdot g_3)$,
- **identity:** $\exists e \in G \; \forall g \in G : e \cdot g = g$
- **invertibility:** $\forall g \in G \; \exists g^{-1} \in G : g^{-1} \cdot g = e$

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Definition (G acts on X)

- **group action:** $G \times X \to X, \quad (g, x) \mapsto g \cdot x$
- **identity:** $e \cdot x = x$
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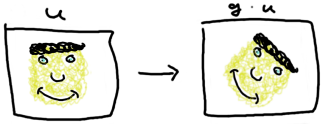
Definition (Equivariance) G acts on X and Y, $\Phi : X \to Y$ is called **equivariant** if for all $g \in G, x \in X$

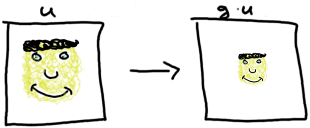
$$g \cdot \Phi(x) = \Phi(g \cdot x)$$

Group actions on functions, e.g. $X = L^2(\mathbb{R}^n, \mathbb{R}^m)$

domain: $(g \cdot u)(x) = u(g^{-1} \cdot x)$

translations, rotations, affine transformations





Example: $G = (\mathbb{R}^n, +)$ may act on X via

- $(g \cdot u)(x) = u(x - g)$
- $(g \cdot u)(x) = u(x \exp(g))$, if $n = 1$

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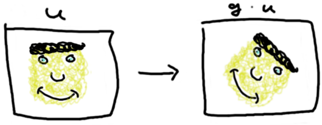

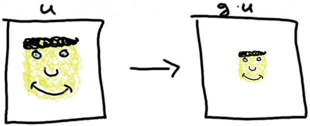

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Example: $G = (\mathbb{R}^m, +)$ may act on X via

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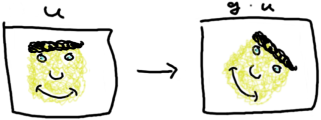

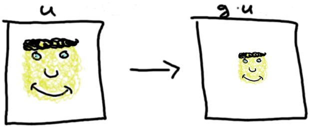

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Example: $G = (\mathbb{R}^m, +)$ may act on X via

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both domain and range: $(g \cdot u)(x) = g \cdot u(g^{-1} \cdot x)$

Acting on domain and range: $(g \cdot u)(x) = g \cdot u(g^{-1} \cdot x)$

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- $\overline{G} = \mathbb{R}^n \rtimes H, \quad H$ subgroup of the general linear group $\mathrm{GL}(n)$
- $g \cdot x = Rx + t, g = (t, R) \in \overline{G}, t \in \mathbb{R}^n, R \in H$
- $\pi : H \to GL(m)$ representation of H
- $(g \cdot u)(x) = \pi(R)u(R^{-1}(x - t))$

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Examples

- **Translations:** $H = \{e\}$
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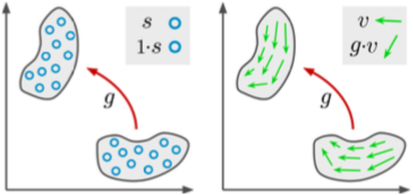
- Example: u vector-field, move and transform vectors



Weiler and Cesa 2019

How to get "equivariant" networks?

Proposition Let G be any group.

- The **composition** $\Phi \circ \Psi$ is equivariant if Φ and Ψ are equivariant.
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Proposition (bias) Let $\Phi : X \to X, (\Phi u)(x) = u(x) + b(x)$. For any group G, Φ is equivariant if b is invariant, i.e. $g \cdot b = b$.

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We can construct $\overline{G}$-equivariant neural networks in the usual way:

- layers $\Phi = \Phi_n \circ \cdots \circ \Phi_1$
- $\Phi(u) = \sigma(Au + b)$
- ResNet $\Phi(u) = u + \sigma(Au + b)$

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In a nutshell: Linear $\overline{G}$-equivariant operators are convolutions with a kernel satisfying an additional constraint.

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Theorem paraphrasing e.g. Weiler and Cesa 2019
Let X, Y be function spaces, e.g. $X = L^2(\mathbb{R}^n, \mathbb{R}^m)$, $Y = L^2(\mathbb{R}^n, \mathbb{R}^M)$. The linear operator $\Phi : X \to Y$,

$$\Phi f(x) = \int K(x, y) f(y) dy$$

with $K : \mathbb{R}^n \to \mathbb{R}^{M \times m}$ is $\overline{G}$-**equivariant** iff there is a k such that

$$\Phi f(x) = \int k(x - y) f(y) dy$$

and k is H-invariant, i.e. for all $R \in H$, $x \in \mathbb{R}^n$: $k(Rx) = k(x)$.

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Let $\psi : \mathbb{R} \to \mathbb{R}$ be any non-linear function.

- **Norm nonlinearity** $\Psi_N : X \to X$,

$$[\Psi_N(u)](x) = u(x) \cdot \psi(\|u(x)\|)$$

- **Pointwise and componentwise nonlinearity** $\Psi_P : X \to X$,

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Lemma Both nonlinearities are $\overline{G}$-equivariant.

Equivariance and inverse problems

- inverse problem $Au = b$, solution operator: $\Phi : Y \to X$
- **Hope** $\Phi \circ A$ is equivariant, e.g. $R_\theta \circ \Phi \circ A = \Phi \circ A \circ R_\theta$

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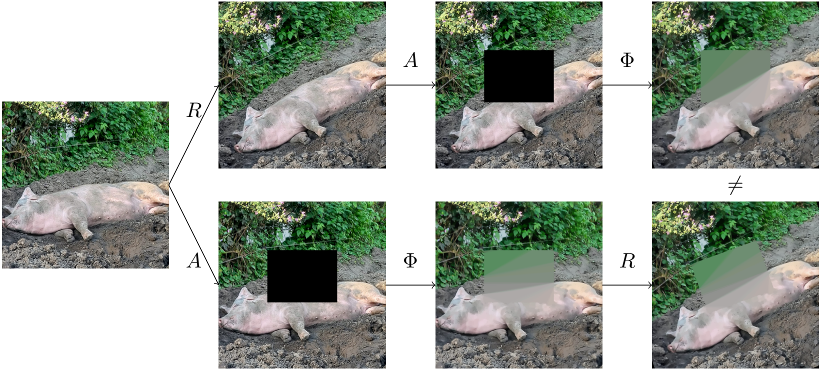
- Even if J is invariant, $\Phi \circ A$ is **not generally equivariant**
- Example: TV and inpainting



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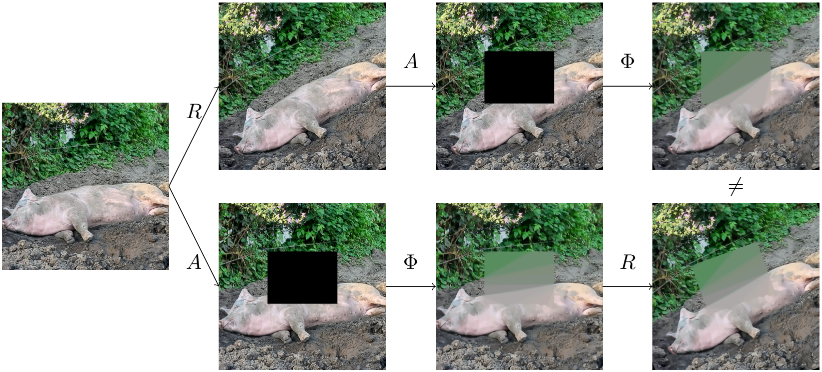

What about well-behaved kernel: compressed sensing?

Invariant functional implies equivariant proximal operator

Theorem Celledoni et al. 2021

- G acts **isometrically** on X ($\|g \cdot u\| = \|u\|$)
- $J : X \to \mathbb{R} \cup \{+\infty\}$ is **invariant** ($J(g \cdot u) = J(u)$)
- J has **well-defined single-valued proximal operator**

Then prox_J is **equivariant**, i.e for all $u \in X$ and $g \in G$

$$\text{prox}_J(g \cdot u) = g \cdot \text{prox}_J(u).$$

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Theorem Celledoni et al. 2021

- G acts **isometrically** on X ($\|g \cdot u\| = \|u\|$)
- $J : X \to \mathbb{R} \cup \{+\infty\}$ is **invariant** ($J(g \cdot u) = J(u)$)
- J has **well-defined single-valued proximal operator**

Then prox_J is **equivariant**, i.e for all $u \in X$ and $g \in G$

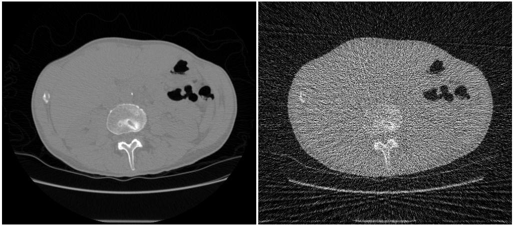
$$\mathrm{prox}_J(g \cdot u) = g \cdot \mathrm{prox}_J(u).$$

- Proof does **generalize** to variatial regularization with L^2-datafit **if** A **is equivariant**
- For **example** the total variation (and higher order variants) is invariant to rigid motion

Numerical Results

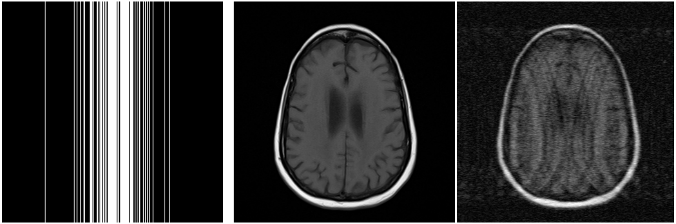
Datasets

- **CT:** LIDC-IDRI data set, 5000+200+1000 images, 50 views



u $\quad$ $\mathrm{FBP}(y)$

- **MR:** FastMRI data set, 5000+200+1000 images



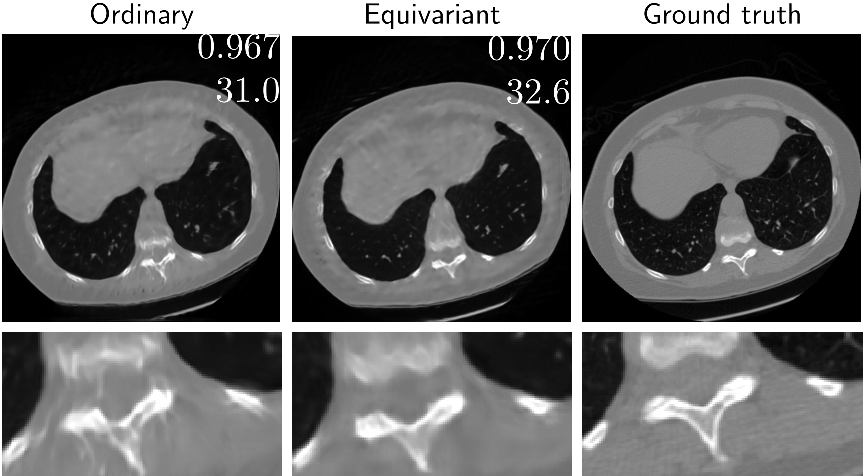
$\mathcal{S}$ $\quad$ u $\quad$ $\mathcal{F}^{-1}(\mathcal{S}^* y)$

CT Results

Equivariant = roto-translations; Ordinary = translations

Equivariant improves upon Ordinary:

- **higher** SSIM and PSNR
- **fewer** artefacts and **finer** details



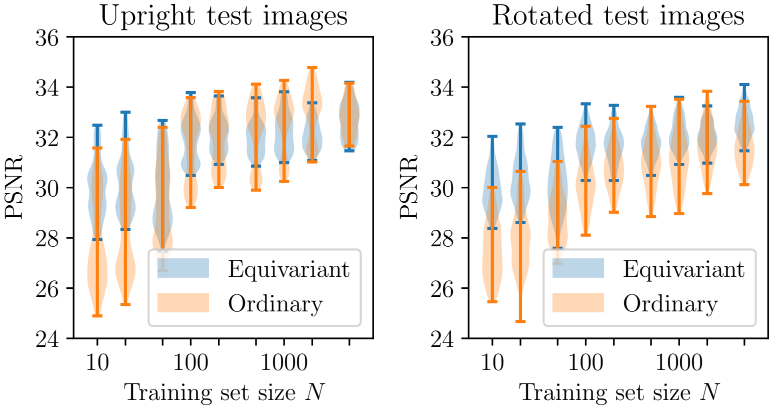
CT Results

Equivariant = roto-translations; Ordinary = translations

Equivariant improves upon Ordinary:

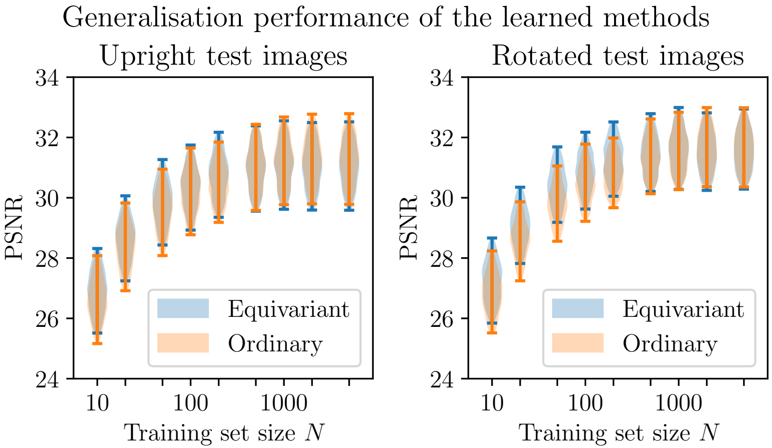
- **small** training sets
- **unseen** orientations

Generalisation performance of the learned methods



MR Results

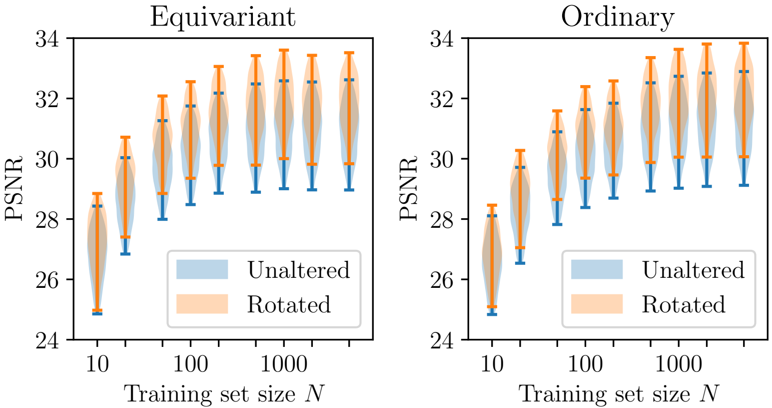
- **similar** observations in MR (as in CT); smaller difference
- results for both methods **better on rotated** images



MR Results: Smoothing

- **smoothing helps:** easier to train on smoother images

Performance of the learned methods on upright images



Conclusions and Outlook

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- **no need for data augmentation**: **mathematically guaranteed** equivariant neural networks exist (though some extra work is needed)
- **solution operators** may **not** be equivariant, but **proximal operators** usually are **equivariant**
- computationally **efficient**: as convolutional networks at run time
- useful for many **applications**: **fewer data** and **robustness**

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Future work

- **other groups**, e.g. scaling of itensities
- **other inverse problems**, e.g. compressed sensing or trivial kernel
- **higher dimensions** e.g. 3D or dynamic inverse problems