# Fast Training of Implicit Networks with Applications in Inverse Problems 

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## Acknowledgements

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## What are Inverse Problems?

Inverse problems consist of recovering a signal $x^{*}$ (e.g. an image, a parameter of a PDE, etc.) from indirect, noisy measurements $d$. This measurement process is usually modeled as an operator $\mathcal{A}$, satisfying the following:

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Our task deals with image deblurring, i.e.,

- $d \in \mathbb{R}^{n \times n}$ : blurred image with noise
- $x^{*} \in \mathbb{R}^{n \times n}$ : original image
- $\varepsilon \in \mathbb{R}^{n \times n}$ : random noise (unknown) in $\mathbb{R}^{n \times n}$


## From a Classical Approach

Direct Inverse:

$$
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Blurred Noisy Image


Apply Inverse


## Classical Approach Cont.

Optimization: Formulate an optimization problem as follows:

$$
x^{*}=\underset{x \in \mathbb{R}^{n \times n}}{\arg \min } \frac{1}{2}\|\mathcal{A} x-d\|_{L^{2}}^{2}+\lambda R(x)
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where $R(x)$ is chosen based on prior knowledge of your data, $\lambda>0$ is a tunable parameter.

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E.g. Use gradient descent where $R(x)=\frac{\lambda}{2}\|x\|_{L^{2}}^{2}$ :

Original Image Blurred Noisy Image Apply Gradient Descent


## Implicit Deep Learning

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- Mimic gradient descent ${ }^{5}$, but replace $\lambda \nabla_{x} R$ with a trainable network $S_{\Theta}$ : $\forall i$ and $0 \leq k \leq K-1$,

$$
x_{i}^{k+1}=\underbrace{x_{i}^{k}-\eta\left(\nabla_{x}\left\|\mathcal{A} x_{i}^{k}-d_{i}\right\|_{L^{2}}^{2}+S_{\Theta}\left(x_{i}^{k}\right)\right)}_{:=T_{\Theta}\left(x_{i}^{k}\right)}
$$

where:

- $\eta>0$ is step size
- $T_{\Theta}(\cdot)$ is a layer of our neural network $\mathcal{N}_{\Theta}(\cdot)$
- $K$ is the number of layers

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- $K$ is the number of layers
- Problems: memory, choice of $K$

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-     - Convergent if $T_{\Theta}(\cdot)$ is a contraction mapping with Lipschitz constant $\gamma \in[0,1)$, i.e, $\forall y_{1}, y_{2} \in \mathbb{R}^{n^{2}},\left\|T_{\Theta}\left(y_{1}\right)-T_{\Theta}\left(y_{2}\right)\right\|_{L^{2}} \leq \gamma\left\|y_{1}-y_{2}\right\|_{L^{2}}$


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Then, by Banach fixed-point theorem, there exists $y^{*} \in \mathbb{R}^{n^{2}}$ s.t. $T_{\Theta}\left(y^{*}\right)=y^{*}$


## Implicit Backpropagation

Suppose we find a fixed point $x^{*}$ for the previous update, i.e.,

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\Longrightarrow & \left(I-\frac{d T_{\Theta}\left(x^{*}\right)}{d x^{*}}\right) \frac{d x^{*}}{d \Theta}=\frac{\partial T_{\Theta}\left(x^{*}\right)}{\partial \Theta} \tag{1}
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\Theta \leftarrow \Theta-\alpha \frac{d \ell}{d x^{*}}\left(I-\frac{d T_{\Theta}\left(x^{*}\right)}{d x^{*}}\right)^{-1} \frac{\partial T_{\Theta}\left(x^{*}\right)}{\partial \Theta}
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where $\alpha>0$ is the learning rate.

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where $\alpha>0$ is the learning rate.
Potential problem: solving (1) is highly nontrivial

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- Implicit Networks calculate the true gradient:

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\nabla_{\Theta} \ell=\frac{d \ell}{d x^{*}}\left(I-\frac{d T_{\Theta}\left(x^{*}\right)}{d x^{*}}\right)^{-1} \frac{\partial T_{\Theta}\left(x^{*}\right)}{\partial \Theta}
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- JFB approximates the gradient: $p_{\Theta}=\frac{d \ell}{d x^{*}} \frac{\partial T_{\Theta}\left(x^{*}\right)}{\partial \Theta}$ which is a descent direction for $\ell$ if the following conditions hold (next slide) ${ }^{6}$ :

[^7]
## JFB Conditions

If:
i. $T_{\Theta}$ is contraction mapping with Lipschitz constant $\gamma$
ii. $T_{\Theta}$ is continuously differentiable w.r.t. $\Theta$
iii. $M:=\frac{\partial T_{\Theta}}{\partial \Theta}$ has full column rank
iv. $M$ is well-conditioned, i.e., $\kappa\left(M^{\top} M\right)<\frac{1}{\gamma}$

Then

$$
p_{\Theta}=\frac{d \ell}{d x^{*}} \frac{\partial T_{\Theta}}{\partial \Theta}
$$

is a descent direction for loss function $\ell$.

## Numerical Experiments

- Dataset: CelebA ${ }^{7}$ (annotated celebrity faces)


[^8]
## Numerical Experiments

- Generate blurred noisy images:



## Numerical Experiments

- Generate blurred noisy images:

- Train with JFB


## Numerical Experiments

- Generate blurred noisy images:


## original image

blurred noisy image

$\mathrm{PSNR}=21.57, \mathrm{SSIM}=0.80$

- Train with JFB
- Preliminary results:

Loss v.s. number of SGD iterations
Reconstructed image


$\mathrm{PSNR}=25.69, \mathrm{SSIM}=0.86$

## Future Work

- Train models using different learned optimization algorithms, e.g. Proximal Gradient Descent and Alternating Directions Method of Multipliers (ADMM)
- Experiment with fastMRI data ${ }^{8}$
- Compare training speeds and accuracy with Jacobian-based algorithms

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Thank you!

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## References

S. Boyd, N. Parikh, E. Chu, B. Peleato, and J. Eckstein. (2011)

Distributed optimization and statistical learning via the alternating direction method of multipliers
Foundations and Trends in Machine Learning 3:1-122, 012011.
S. Boyd and L. Vandenberghe (2004)

Convex Optimization
Cambridge University Press
Z. Liu, P. Luo, X. Wang, and X. Tang (2015)

Deep learning face attributes in the wild
Proceedings of the IEEE international conference on computer vision 3730-3738, 2015
目
C. Vogel (2002)

Computational Methods for Inverse Problems
Frontiers in Applied Mathematics. Society for Industrial and Applied
Mathematics

## References Cont．

固
S．W．Fung，H．Heaton，Q．Li，D．McKenzie，S．Osher，and W．Yin（2021） Jfb ：Jacobian－free back－propagation for implicit networks．
arXiv preprint arXiv：2103．12803
R D．Gilton，G．Ongie，and R．Willett．（2021）
Deep equilibrium architectures for inverse problems in imaging． IEEE Transactions on Computational Imaging 7：1123－1133

宔
G．Ongie，A．Jalal，C．A．Metzler，R．G．Baraniuk，A．G．Dimakis，and R． Willett（2020）
Deep learning techniques for inverse problems in imaging IEEE Journal on Selected Areas in Information Theory 1（1）：39－56
R S．Bai，J．Z．Kolter，and V．Koltun．D（2019）
Deep equilibrium models
Advances in Neural Information Processing Systems 32
䬎
J．Zbontar，F．Knoll，A．Sriram，T．Murrell，Z．Huang，M．J．Muckley，A．
Defazio，R．Stern，P．Johnson，M．Bruno，et al．（2018）
fastmri：An open dataset and benchmarks for accelerated mri
arXiv preprint arXiv：1811．08839， 2018.

## Banach Fixed-Point Theorem

We demonstrate it in $\mathbb{R}^{d}$ :
Suppose $T: \mathbb{R}^{d} \mapsto \mathbb{R}^{d}$ is a contraction map with Lipschitz constant $\gamma \in[0,1)$.
$\forall x_{0} \in \mathbb{R}^{d}$, iterate as follows:

$$
\begin{gathered}
x_{1}=T\left(x_{0}\right) \\
x_{2}=T\left(x_{1}\right) \\
\vdots \\
x_{i+1}
\end{gathered}=T\left(x_{i}\right)
$$

Then we obtain a sequence $\left\{x_{m}\right\}_{m \in \mathbb{N}}$

## Banach Fixed-Point Theorem

Observe that

$$
\begin{aligned}
\left\|x_{2}-x_{1}\right\| & =\left\|T\left(x_{1}\right)-T\left(x_{0}\right)\right\| \leq \gamma\left\|x_{0}-x_{1}\right\| \\
\left\|x_{3}-x_{2}\right\| & =\left\|T\left(x_{2}\right)-T\left(x_{1}\right)\right\| \leq \gamma\left\|x_{2}-x_{1}\right\| \leq \gamma^{2}\left\|x_{0}-x_{1}\right\| \\
& \vdots \\
\left\|x_{i+1}-x_{i}\right\| & \leq \gamma^{i}\left\|x_{0}-x_{1}\right\|
\end{aligned}
$$

So $\lim _{m \rightarrow \infty}\left\|x_{m+1}-x_{m}\right\| \leq \lim _{m \rightarrow \infty} \gamma^{m}\left\|x_{0}-x_{1}\right\|=0$
We also know that $0 \leq \lim _{m \rightarrow \infty}\left\|x_{m+1}-x_{m}\right\|$.
$\Longrightarrow \lim _{m \rightarrow \infty}\left\|x_{m+1}-x_{m}\right\|=0$ by Squeeze Theorem

## Banach Fixed-Point Theorem

By Triangular Inequality,

$$
\begin{aligned}
\left\|x_{m+k}-x_{m}\right\| & \leq\left\|x_{m}-x_{m+1}\right\|+\left\|x_{m+1}-x m+k\right\| \\
& \leq\left\|x_{m}-x_{m+1}\right\|+\left(\left\|x_{m+1}-x_{m+2}\right\|+\left\|x_{m+2}-x_{m+k}\right\|\right) \\
& \vdots \\
& \leq\left\|x_{m}-x_{m+1}\right\|+\left\|x_{m+1}-x_{m+2}\right\|+\cdots \\
& +\left\|x_{m+k-2}-x_{m+k-1}\right\|+\left\|x_{m+k-1}-x_{m+k}\right\|
\end{aligned}
$$

By Squeeze Theorem again, $\left\{x_{m}\right\}_{m \in \mathbb{N}}$ is a Cauchy sequence, which is equivalent to $\lim _{m \rightarrow \infty} x_{m}=x^{*}$ exists.
$\Longrightarrow x^{*}=T\left(x^{*}\right)$ is a fixed point.


## Proximal Gradient Descent

With a function $h(\cdot)$, we can define a proximal operator

$$
\operatorname{prox}_{h}(x)=\underset{u}{\arg \min } \frac{1}{2}\|u-x\|_{L^{2}}^{2}+h(u)
$$

Then the updating rule becomes:

$$
x^{k+1}=\operatorname{prox}_{h, \eta}\left(x^{k}-\eta \nabla_{x}\left\|\mathcal{A} x^{k}-d\right\|_{L^{2}}^{2}\right)
$$

We can replace this prox ${ }_{h}$ with a trainable network $R_{\Theta}(\cdot)$ :

$$
x^{k+1}=R_{\Theta}\left(x^{k}-\eta \nabla_{x}\left\|\mathcal{A} x^{k}-d\right\|_{L^{2}}^{2}\right)
$$


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[^1]:    ${ }^{5}$ Davis Gilton, Gregory Ongie, and Rebecca Willett. "Deep equilibrium architectures for inverse problems in imaging." IEEE Transactions on Computational Imaging 7 (2021): 1123-1133.

[^2]:    ${ }^{5}$ Davis Gilton, Gregory Ongie, and Rebecca Willett. "Deep equilibrium architectures for inverse problems in imaging." IEEE Transactions on Computational Imaging 7 (2021): 1123-1133.

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[^9]:    ${ }^{8}$ Zbontar, Jure, et al. "fastMRI: An open dataset and benchmarks for accelerated MRI." arXiv preprintiarXiv:1811.08839 (2018).

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