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Splitting Algorithms and

Generalized Normalizing Flows

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Lectures

- 0. Motivation
- 1. Splitting Algorithms
- 2. Optimal Transport and SMART
- 3. Normalizing Flows
- 4. Generalized Normalizing Flows

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Motivation: Inverse Problems in Imaging





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79	83	95	115	134	141	137	101	91	114

Visual system: Checkerboard shadow illusion of Adelson



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Other Images

Color images: Many color systems, e.g. RGB system from computer screen, HSV ...



Visual system: Illustration of the lateral inhibition (Courtesy: M. Bertalmio)



Hyperspectral images:



Manifold-values images: DT-MRI, IN-SAR



Images on \mathbb{R}^3 and manifolds:





Motivation: Inverse Problems in Imaging

Inverse Problem: Find x given y with (known/unknown) forward operator F,

 $y = \operatorname{noisy}(F(x))$

Find solution as minimizer of variational model:

$$\mathcal{J}(x) = \underbrace{\mathcal{D}_F(x, y)}_{\text{data term}} + \lambda \underbrace{\mathcal{R}(x)}_{\text{regularizer, prior}}, \qquad \lambda >$$

0

Examples:

- image restoration: denoising, (blind) deblurring, inpainting, superresolution,
- computerized tomography (CT) (Video Siltanen)
- MRI (Fouriermatrix)
- ◆ FIB: Focused ion beam
- EBSD: Electron backscatter diffraction ($\mathcal{M} = \mathrm{SO}(3)/\mathcal{S}$)
- diffraction tomography
- SMLM: single molecule localization microscopy



- Regularizer to make the problem well-posed, since F is in general ill-posed/ill-conditioned
 - F(x) = y has no solution (PCA)
 - no unique solution (inpainting)
 - solution does not depend continuously on input data (compact operators, deblurring, CT) mildly ill-posed $\sigma_n > Cn^{-\gamma}$, $\gamma \leq 1$, moderately ill-posed $\sigma_n > Cn^{-\gamma}$, $\gamma > 1$, severely ill-posed singular values decay faster than polynomial speed

Prior for certain class of images: Bayesian (MAP) approach

$$\hat{x} \in \underset{x}{\operatorname{argmax}} \log \left(p_{X|Y=y}(x) \right) \qquad \text{Bayes: } p_{X|Y=y}(x) = \frac{p_{Y|X=x}(y)p_{Y}(y)}{p_{X}(x)}$$
$$= \underset{x}{\operatorname{argmin}} \left\{ -\log \left(p_{Y|X=x}(y) \right) - \log \left(p_{X}(x) \right) \right\}$$
$$= \underset{x}{\operatorname{argmin}} \left\{ \underbrace{\mathcal{D}_{F}(x,y)}_{\text{data-fidelity term}} + \lambda \underbrace{\mathcal{R}(x)}_{\text{prior}} \right\}$$

e.g. Gibbs prior

$$p_X(x) = e^{-\lambda \mathcal{R}(x)} \in L_1(\mathbb{R}^d)$$

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Typical regularizer/prior:

- Tikhonov regularizer:
 - continuous: $\mathcal{R}(u) = \int_{\Omega} |\nabla u|^2 \,\mathrm{d} oldsymbol{x} = |u|^2_{W^1_2}$
 - discrete: $\mathcal{R}(x) = \| |\nabla x|^2 \|_1 = \sum_{i,j} (x_{i+1,j} x_{i,j})^2 + (x_{i,j+1} x_{i,j})^2$
- Total Variation regularization:
 - continuous: $\mathcal{R}(u) = |Du|_{TV} = \sup_{\varphi \in C_c^1(\Omega, \mathbb{R}^2), \|\varphi\|_{\infty} \leq 1} \langle u, \operatorname{div} \varphi \rangle = |u|_{W_2^1}$
 - discrete: $\mathcal{R}(x) = \| |\nabla x| \|_1 = \sum_{i,j} \sqrt{(x_{i+1,j} x_{i,j})^2 + (x_{i,j+1} x_{i,j})^2}$



$$\underset{x}{\operatorname{argmin}} \left\{ \frac{1}{2} \|y - x\|^2 + \lambda \mathcal{R}(x) \right\}$$

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MAP Estimation



Right: Phantom of a confocal microscopy image illustrating a neuron. Middle: white additive Gaussian noise Right: Poisson noise (Courtesy: A. Jezierska, PhD thesis)

•
$$\operatorname{argmin}_{x} \left\{ -\log\left(p_{Y|X=x}(y)\right) - \log\left(p_{X}(x)\right) \right\}$$

$$p_{Y|X=x}(y) = \begin{cases} \frac{1}{(2\pi\sigma^2)^{N/2}}e^{-\frac{\|y-F(x)\|_2^2}{2\sigma^2}} & \text{Gaussian noise,} \\ \prod_{i=1}^N \frac{(F(x)_i)^{y_i}e^{-F(x)_i}}{y_i!} & \text{Poisson noise} \end{cases}$$

Up to a constant

$$-\log\left(p_{Y|X=x}(y)\right) = \begin{cases} \frac{1}{2\sigma^2} \|y - F(x)\|_2^2 & \text{Gaussian,} \\ -\sum_i y_i \log(F(x)_i) + F(x)_i = \mathrm{KL}(y, F(x)) + c & \text{Poisson} \end{cases}$$

with Kullback-Leibler divergence (componentwise)

$$\mathrm{KL}(u, v) = u \log u - u \log v - u + v$$

Example 1: Removal of Curtaining Effects in FIB



Model:

$$\mathcal{J}(u, s, l) = \|f - (u + s + l)\|_2^2 + \varphi_1(u) + \varphi_2(s) + \varphi_3(l),$$

with

$$\begin{split} \varphi_1(u) &:= & \mu_1 \| \nabla_{x,z} u \|_{2,1} + \mu_2 \| \Delta_z u \|_1 + \iota_{[0,1]^N}(u), \\ \varphi_2(s) &:= & \| \nabla_y s \|_1, \\ \varphi_3(l) &:= & \mu_3 \| \nabla_{x,y} l \|_{2,1} \end{split}$$

Video: J.-H. Fitschen

Example 2: Strain Computation



Top: Experimental setup for the tensile test inside a scanning electron microscope. Bottom: Load-deformation diagram with three selected micrographs taken under increasing load.

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Example 2: Strain Computation

Model: $u = (u_1, u_2)^{\mathsf{T}}$ vector field

$$\mathcal{J}(u) := \|A_{f_2}u + c_{f_1, f_2}\|_1 + \mathrm{TGV}(u)$$

where the data term arises from linearizing the brightness invariance assumption:

$$0 \approx f_1(x) - f_2(x + u(x)) \\ \approx f_1(x) - f_2(x + \bar{u}(x)) - \left\langle \nabla f_2(x + \bar{u}(x), u(x) - \bar{u}(x) \right\rangle$$

and the regularizer is

$$\mathrm{TGV}(u) := \inf_{a} \left\{ \int_{\Omega} \lambda_1 \underbrace{\|\nabla u - a\|_F}_{\text{local feature}} + \lambda_2 \underbrace{\|\nabla a\|_F}_{\text{global feature}} dx \right\}$$

Reference: Bredies, Kunisch, Pock 2010, Setzer, Steidl 2008

Example 2: Strain Computation





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- MSE: $MSE(u, f) := \frac{1}{N} ||u f||_2^2$
- PSNR: Peak signal to noise ratio $PSNR(u, f) := 10 \log_{10} \frac{|\max f \min f|^2}{\frac{1}{N} ||u f||_2^2}$,
- MAE: Mean absolute error $MAE(u, f) := \frac{1}{N} ||f u||_1$.
- SSIM: Structure similarity measure (Simoncelli et al. 2004)
- Sharpness index (Moisan et al. 2011)
- LPIPS: Learned Perceptual Image Patch Similarity (Zhang/Efros 2018)



Different type of distortions, all with MSE = 210. (a) Original image, (b) Contrast-stretched image, SSIM = 0.9168, (c) Mean-shifted image, SSIM = 0.9900, (d) JPEG compressed image, SSIM = 0.6949, (e) Blurred image, SSIM = 0.7052, (f) Salt-pepper noise contaminated image, SSIM = 0.7748. Image: Simoncelli et al 2004.



Motivation: Neural Networks and Deep Learning

M. Elad (2017) SIAM News: **Deep, deep trouble**: Deep learning's impact on image processing, mathematics, and humanity Change to: **High, high challenge**



NN: $\Phi(\cdot; \theta) : \mathbb{R}^d \to \mathbb{R}^{n_K}$ of the form

$$\Phi\left(\cdot;\theta\right):=A_{K}\sigma\circ A_{K-1}\sigma\circ\ldots\sigma\circ A_{1}$$

with non-linear activation $\sigma \colon \mathbb{R} \to \mathbb{R}$ acting componentwise and affine functions

$$A_k(x) := W_k x + b_k, \qquad W_k \in \mathbb{R}^{n_k, n_{k-1}}, \ b_k \in \mathbb{R}^{n_k}$$

Training of a NN by minimizing

$$\mathcal{J}(heta) := \sum_{i=1}^N \ell ig(\Phi(x_i; heta); y_i ig),$$

Minimization Algs: stoch. gradient descent algorithm (filtered backprojection, automatic differentiation), inertial stoch. PALM Refs: Hertrich/Steidl 2022 Fitschen: ,,most stupid method to solve problems"

Example 1: Deblurring

Helsinki Deblur Challenge 2021 organized by the Finish Inverse Problem Society

Winner: Genzel, MacDonald, März (PhD), T. Trippe (Master thesis) TUB

• Goal: deblurring of text images obtained by an optical aperture



20 levels of increasing defocus blur, 200 samples per level

• Results:

ZJXDGCiruE KrextmkKeC gSvmJmJEKE	ZJXDGCiruE KrextmkKeC gSvmJmJEKE	organal characters 2005Gin/E Krestericoc 65w0v0002 003_scanc 108.0	TF2ATuNQE2 jaxigiuAhg PwyPtinTagiO	TFzATuNQEz jaxigiuNhg PwyPYnTapD	original charactors: TrietTuyOtz junichAfrie ProyffintTapD OCIL_science 108-0	zM bisrpeJ UgEEAuDJrT LmfiQAtsV	organi charadaysi petingal uptologyy DOR, azaw: \$8.0
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Example 2: Photo Integrated Circuit Design

Master thesis C. Wittmann (with Hertz Institute Berlin)



LPIPS as loss function



End of Motivation

How to model and minimize variational models in inverse problems and how NNs can be incorporated?

Let's do some MATH.

A. Maslow (1966):"If the only tool you have is a hammer, you treat everything as if it were a nail."

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(a) Phantom.



(b) Gaussian noise.



(c) Poisson noise















Elongation in µm





Elongation in µm





























(b)



(a)











Figure 1: Model of a NN with three hidden layers, i.e., d = 4, K = 4, $n_1 = n_2 = n_3 = 5$, $n_4 = 1$.




ZJXDGCiruE KrextmkKeC gSvmJmJEKE	ZJXDGCiruE KrextmkKeC gSvmJmJEKE	original characters: ZIXDGCinuE KreatmkKeC gSvm0m0EKE OCR_score: 100.0	TF2ATuRIQE2 jaxigiumhg PwyPrinTagiO	TFzATuNQEz jaxigiuNhg PwyPYnTapD	original characters: TF2ATuNQEz joxigiuNng PwyPYnTapD OCR_score: 100.0	zM bisrpeJ UgEEAuDJrT LmfiQAtsV	onginal characters: 2M bisme1 UgEEAuDIrT LmfQAtsv OCR_scure: 90.0
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cXF XfnuLM ueBwRquMYc vpSYztfNTM	cXF XfnuLM ueBwRquMYc vpSYztfNTM	original characters: cXF XfnuLM ueiBwHquMYc vpSYzthNTM OCR_score: 90.0	märgenriksjä gärmonivoltes obs. settensä	mZrgnyULjJ gjSmxAvcNe sSh AfFWsf	original characters : m2rgnvLLJ gjSmxAvcNe sSh AFTWsf OCR_score: 100.0	SutLMcqJsB asqrmfVyqh gvE bmrnMQt	onginal characters: Sutt McqJsB asgrmfVygh gvE bmmMQt OCR_score: 100.0
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