Efficient generative models for computational imaging

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arXiv 2406.02462
arXiv 2406.10211

Overview

$$\underbrace{\text{Efficient}}_{\text{III}}\ \underbrace{\text{generative models}}_{\text{II}}\ \text{for}\ \underbrace{\text{computational imaging}}_{\text{I}}$$

Dall·E 3's view of this talk I



Dall·E 3's view of this talk II

Outline

Image deblurring

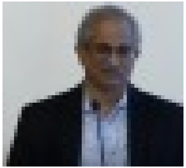
measurement $\boldsymbol{y}$

→ CI algorithm →

estimate $\hat{\boldsymbol{x}}$

Image super-resolution

measurement $\boldsymbol{y}$



$\rightarrow$ CI algorithm $\rightarrow$

estimate $\hat{\boldsymbol{x}}$

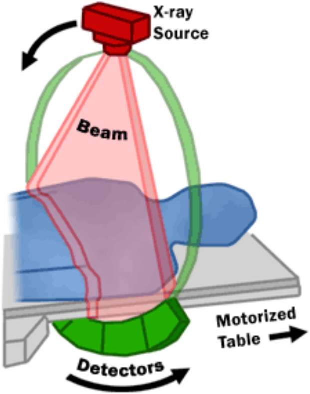
measurement $\boldsymbol{y}$

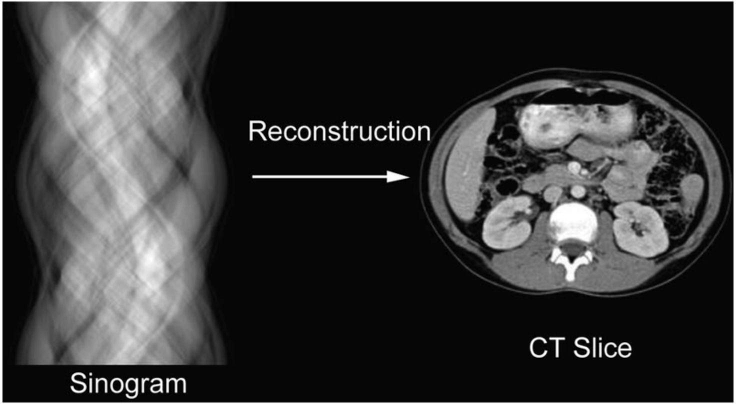
(missing pixel values)

$\rightarrow$ CI algorithm $\rightarrow$

estimate $\hat{\boldsymbol{x}}$

X-ray computed tomography (CT)

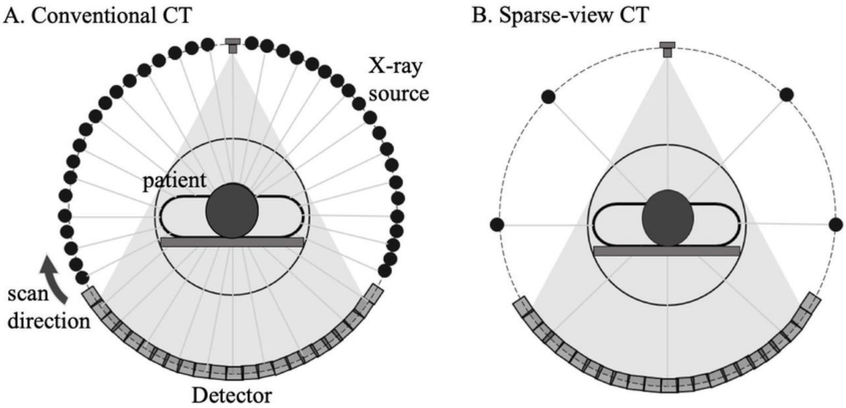




measurement $\boldsymbol{y}$ estimate $\hat{\boldsymbol{x}}$

Left image from FDA Right image from [1]

Sparse-view X-ray CT reduces radiation dose



Lower dose, but now a highly under-determined inverse problem [2].

Under-determined inverse problems

- Applications: compressed sensing MRI, sparse-view CT, inpainting, ...
  All have *linear* forward models for data:

$$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{\varepsilon}$$

  $\boldsymbol{y}$: sensor data (*e.g.*, sinogram)
  $\boldsymbol{A}$: wide system matrix (known)
  $\boldsymbol{x}$: latent image (or image series in dynamic problems)
  $\boldsymbol{\varepsilon}$: noise with known distribution provides likelihood $\mathrm{p}(\boldsymbol{y}|\boldsymbol{x})$
- Maximum-likelihood estimation (physics-based fitting) is usually non-unique:

$$\hat{\boldsymbol{x}} = \arg\max_{\boldsymbol{x}} \log \mathrm{p}(\boldsymbol{y}|\boldsymbol{x}) = \underbrace{\arg\min_{\boldsymbol{x}} \|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{y}\|_2^2}_{\text{(for gaussian noise)}}$$

- Minimum-norm least-squares solution is unique but usually impractical or useless:

$$\hat{\boldsymbol{x}} = \boldsymbol{A}^{+}\boldsymbol{y} = \boldsymbol{y} \text{ for inpainting problem}$$

Inverse problem solution methods

- hand-crafted regularizers

$$\hat{\boldsymbol{x}} = \arg\min_{\boldsymbol{x}} -\log \mathrm{p}(\boldsymbol{y}|\boldsymbol{x}) + R(\boldsymbol{x}) = \arg\min_{\boldsymbol{x}} \frac{1}{2\sigma_\varepsilon^2} \|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{y}\|_2^2 + R(\boldsymbol{x})$$

- black-box data-driven supervised methods:

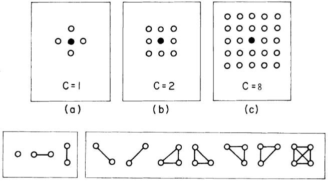
$$\boldsymbol{A}^+ \boldsymbol{y} \to \boxed{\text{NN}} \to \hat{\boldsymbol{x}}$$

- unrolled deep learning methods (PNP, RED, MoDL, ...)
- Bayesian methods (*e.g.*, MAP) based on a prior $\mathrm{p}(\boldsymbol{x})$, lately (?) relabeled as generative models

Long history of Bayesian models for inverse problems

Markov random field models

(*e.g.*) Geman & Geman 1984 [3]



Mostly for inference?

GEMAN AND GEMAN: STOCHASTIC RELAXATION, GIBBS DISTRIBUTIONS, AND BAYESIAN RESTORATION 737

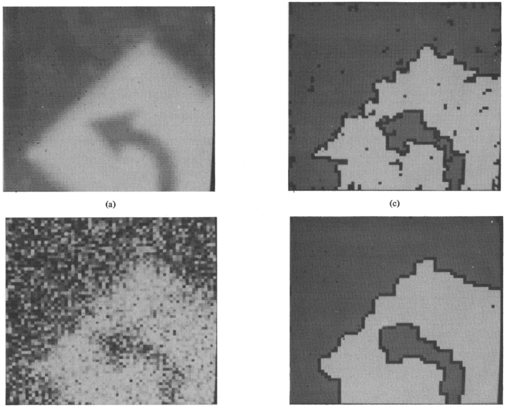


Fig. 7. (a) Blurred image (roadside scene). (b) Degraded image: Additive noise. (c) Restoration including line process; 100 iterations. (d) Restoration including line process; 1000 iterations.

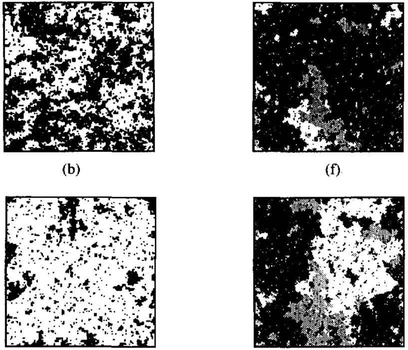
MRF as generators?

[4] T-PAMI 1994

An Empirical Study of the Simulation of Various Models Used for Images

A. J. Gray, J. W. Kay, and D. M. Titterington

Abstract— Markov random fields are typically used as priors in Bayesian image restoration methods to represent spatial information in the image. Commonly used Markov random fields are not in fact capable of representing the moderate-to-large scale clustering present in naturally occurring images and can also be time consuming to simulate,



(b) (f) (c) (g)

Local vs global priors

Gray, Kay, Titterington [4] T-PAMI 1994

> *... the local properties of spatial Markov models are undoubtedly plausible descriptors of the local associations typical of many images, which is the way in which the models are often used. Nevertheless, it would be reassuring if models used as priors did in fact provide a realistic representation of our prior assumptions and if their (empirical) properties were more widely known.*

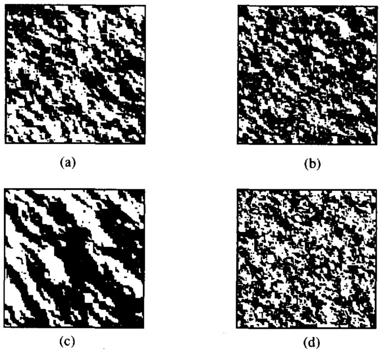
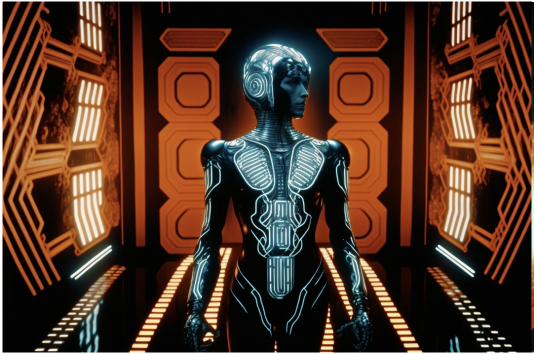


Fig. 4. Realizations of two-dimensional, one-parameter, autologistic Markov Mesh models: (a) binary, second-order model with $\beta = \log 5$; (b) three-color second-order model with $\beta = \log 5$; (c) binary second-order model with $\beta = \log 10$; (d) binary second-order model with $\beta = \log 3$.

Generative models are hot in graphics

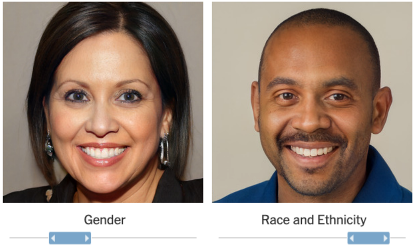
Computer ("AI") generated stills from hypothetical movie: Chilean director Alejandro Jodorowsky's 1976 version of "Tron" using midjourney.com as reported in 2023-01-13 NY Times article "This film does not exist" by director Frank Pavich.

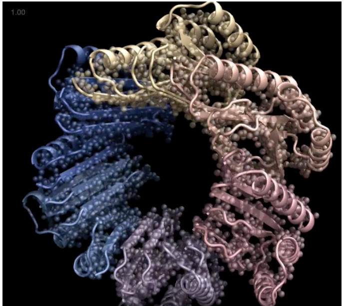
Generative models are hot in the news

- 2020-11-21 NY Times "Designed to Deceive: Do These People Look Real to You?"
  Article about generated (aka fake) faces.

- 2022-10-21 NY Times "A Coming-Out Party for Generative A.I., Silicon Valley's New Craze" (about "Stable Diffusion" image generator)
  `https://nyti.ms/3SjsN0k`

- 2023-01-09 NY Times "A.I. Turns Its Artistry to Creating New Human Proteins"
  `https://nyti.ms/3IzY66m`





Théâtre d'Opéra Spatial

Image created with Midjourney generative AI by Jason M. Allen.

Won 2022 Colorado State Fair fine art competition.

Wikimedia: "This file is in the public domain because it is the work of a computer algorithm or artificial intelligence and does not contain sufficient human authorship to support a copyright claim."

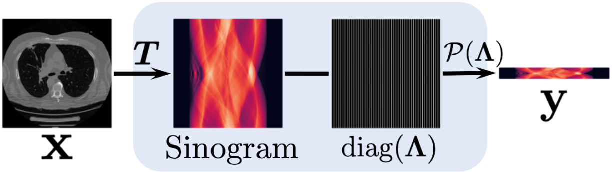
Zhao, Ye, Bresler: Jan. 2023 IEEE SpMag survey paper [5]

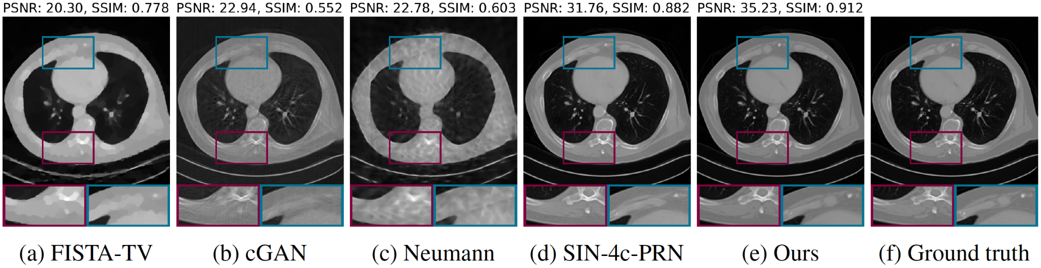
- Generative adversarial network (GAN) models
- Variation auto-encoder (VAE) models [6]
- Normalizing flows [7, 8]
- Score-based diffusion models
  - Zaccharie Ramzi et al., NeurIPS Workshop 2020 [9]
  - Yang Song & Liyue Shen et al., NeurIPS Workshop 2021, ICLR 2022 [10, 11]
  - Ajil Jalal et al. ... Jon Tamir, NeurIPS 2021 [12]
  - Hyungjin Chung & Jong Chul Ye, MIA, Aug. 2022 [13]
  - Luo et al., MRM, 2023 [14]
  - ...
- Kazerouni et al. [15] have github catalog, including >20 (!) survey papers
- ... (hopelessly incomplete lists)

From Song & Shen et al., ICLR 2022 [11].

Trained with 47K 2D images; 23 projection views (≈ 17-fold dose reduction)

$$A = \mathcal{P}(\Lambda)T$$





- Bayesian inference methods use the posterior:

$$\mathrm{p}(\boldsymbol{x}|\boldsymbol{y}) = \underbrace{\mathrm{p}(\boldsymbol{y}|\boldsymbol{x})}_{\text{physics}} \; \underbrace{\mathrm{p}(\boldsymbol{x})}_{\text{prior}} \; / \; \mathrm{p}(\boldsymbol{y})$$

- Here the prior $\mathrm{p}(\boldsymbol{x})$ is for quantifying (prior) probability, not necessarily for generation.
- A model for the posterior $\mathrm{p}(\boldsymbol{x}|\boldsymbol{y})$ opens many doors:
  - Maximizing $\mathrm{p}(\boldsymbol{x}|\boldsymbol{y})$ is maximum a posteriori (MAP) estimation
  - The conditional mean $\mathrm{E}[\boldsymbol{x}|\boldsymbol{y}] = \int \boldsymbol{x} \, \mathrm{p}(\boldsymbol{x}|\boldsymbol{y}) \, \mathrm{d}\boldsymbol{x}$ is the MMSE estimator
  - Sampling from the posterior $\mathrm{p}(\boldsymbol{x}|\boldsymbol{y})$ facilitates uncertainty quantification in inference
- All these methods require the prior $\mathrm{p}(\boldsymbol{x})$, *i.e.*, a prior model $\mathrm{p}(\boldsymbol{x}; \boldsymbol{\theta})$.
-

Bayesian methods (generative models)

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- All these methods require the prior $\mathrm{p}(\boldsymbol{x})$, *i.e.*, a prior model $\mathrm{p}(\boldsymbol{x}; \boldsymbol{\theta})$.
- Or do they?

Sampling via Langevin dynamics

Sampling from a *prior* $\mathrm{p}(\boldsymbol{x}; \boldsymbol{\theta})$ just needs its score function $\nabla_{\boldsymbol{x}} \log \mathrm{p}(\boldsymbol{x}; \boldsymbol{\theta})$, using Langevin dynamics, aka stochastic gradient ascent of log-prior:

$$\boldsymbol{x}_t = \boldsymbol{x}_{t-1} + \alpha_t \underbrace{\nabla \log \mathrm{p}(\boldsymbol{x}_{t-1}; \boldsymbol{\theta})}_{\text{score function}} + \beta_t \mathcal{N}(\mathbf{0}, \boldsymbol{I}), \quad t = 1, \ldots, T.$$

- Draws samples from $\mathrm{p}(\boldsymbol{x}; \boldsymbol{\theta})$ for suitable choices of $\{\alpha_t\}$, $\{\beta_t\}$, and (large) T [16].
- If $\alpha_t = 0$ and $\beta_t = \beta$, then akin to (isotropic) diffusion or Brownian motion

Distribution learning vs score learning

- Typical distribution models: $\mathrm{p}(\boldsymbol{x}; \boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})} \, \mathrm{e}^{-U(\boldsymbol{x}; \boldsymbol{\theta})}$.
  Goal: learn $\boldsymbol{\theta}$ from training data $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_T$
- For IID samples $\{\boldsymbol{x}_t\}$, one could try to learn $\boldsymbol{\theta}$ by ML estimation:

$$\hat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}} \mathrm{p}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_T; \boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \sum_{t=1}^{T} \log(\mathrm{p}(\boldsymbol{x}_t; \boldsymbol{\theta}))$$
$$= \arg\max_{\boldsymbol{\theta}} \left(-T \, {\color{red} Z(\boldsymbol{\theta})} + \sum_{t=1}^{T} -U(\boldsymbol{x}_t; \boldsymbol{\theta}) \right) .$$

  Typically intractable due to the partition function $Z(\boldsymbol{\theta})$.
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  Typically intractable due to the partition function $Z(\boldsymbol{\theta})$.
- In contrast, the score function is easier to handle:

$$\boldsymbol{s}(\boldsymbol{x};\boldsymbol{\theta}) \triangleq \nabla_{\boldsymbol{x}} \log \mathrm{p}(\boldsymbol{x};\boldsymbol{\theta}) = \nabla_{\boldsymbol{x}} \left(-\log Z(\boldsymbol{\theta}) - U(\boldsymbol{x};\theta)\right) = -\nabla_{\boldsymbol{x}} U(\boldsymbol{x};\theta).$$

Score matching

- Given training data $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_T$, learn score function $\boldsymbol{s}(\boldsymbol{x}; \boldsymbol{\theta}) \stackrel{?}{=} \nabla_{\boldsymbol{x}} \log \mathrm{p}(\boldsymbol{x}; \boldsymbol{\theta})$
-

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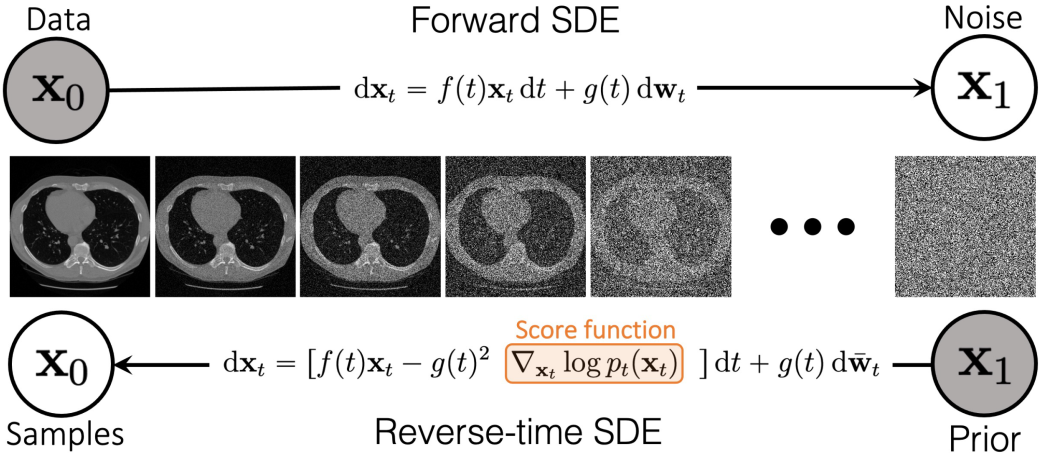
- Explicit score matching (ESM) (Hyvärinen, 2005 [17])
- Implicit score matching (ISM)
- Denoising score matching (DSM) (Vincent, 2011 [18])
- Noise-conditional score matching (NCSM) (Song, 2019 [19, eqn. (5)]):

$$\ell(\boldsymbol{\theta}; \sigma) \triangleq \frac{1}{2} \mathrm{E}_{\mathrm{q}_0(\boldsymbol{x})}\left[\mathrm{E}_{g_\sigma(\boldsymbol{z})}\left[\left\|\boldsymbol{s}(\boldsymbol{x}+\boldsymbol{z}; \boldsymbol{\theta}, \sigma) + \frac{\boldsymbol{z}}{\sigma^2}\right\|_2^2\right]\right], \quad \mathcal{L}(\boldsymbol{\theta}; \{\sigma_l\}) = \frac{1}{L} \sum_{l=1}^{L} \sigma_l^2 \, \ell(\boldsymbol{\theta}; \sigma_l),$$

  where $\boldsymbol{s}(\boldsymbol{x}; \boldsymbol{\theta}, \sigma)$ denotes a *noise-conditional score network* (NCSN).
- $\boldsymbol{d}(\boldsymbol{x}; \boldsymbol{\theta}) \triangleq \boldsymbol{x} + \sigma^2 \boldsymbol{s}(\boldsymbol{x}; \boldsymbol{\theta}, \sigma)$: equivalent image denoiser by Tweedie's formula [20]
- Recommended choice [21]: $\boldsymbol{s}(\boldsymbol{x}; \boldsymbol{\theta}, \sigma) \triangleq \tilde{\boldsymbol{s}}(\boldsymbol{x}; \boldsymbol{\theta})/\sigma$, where $\tilde{\boldsymbol{s}}$ is unitless

Shen & Song et al., NeurIPS 2021 [10]



Score-based diffusion models: trade-offs

- No adversarial training needed
- High quality sample generation (if enough training data)
-

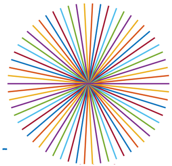
Score-based diffusion models: trade-offs

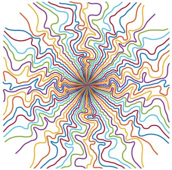
- No adversarial training needed
- High quality sample generation (if enough training data)
- Expensive sample generation (vs GAN models)
  - Distillation methods [22]
  - Consistency models [23]
  - Geometric decomposition [24]
  - Multi-scale [25, 26] and pyramidal [27] and coarse-to-fine [28] models
  - Faster ODE solvers [29]
  - Warm starts [30]
  - Latent diffusion models: use VAE and diffuse in latent space [31–33]. Used in Stable Diffusion by start-up Stability AI
  - 3D image reconstruction using 2D models [34, 35]
- Learning 3D (or 3D+T) whole-image generative models is challenging (training data, GPU memory, ...)

Whole images vs patches?

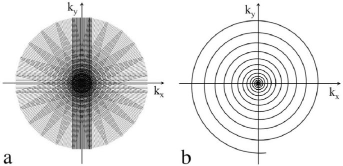
Jan. 2023 survey paper on generative models [5] does not mention “patch” once!?

MRI k-space sampling:

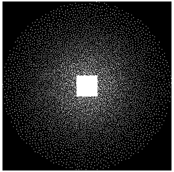




[36]



[37]



[38]

Patch-based models have long history in inverse problems, *e.g.*,

- patch GAN [39–41]
- patch dictionary models [42, 43]
- non-local means, BM3D
- Wasserstein patch prior [44, 45] . . .

Motivating questions

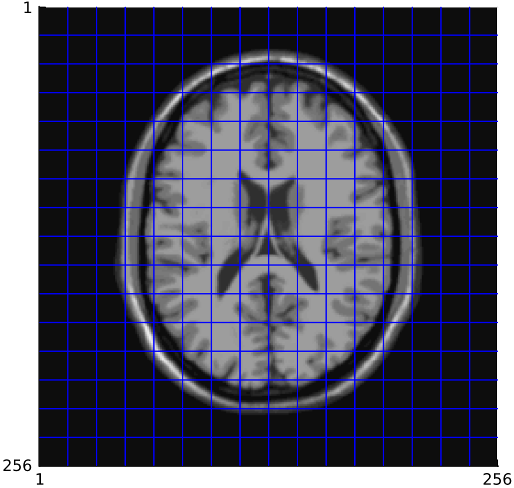
- Could patch-based generative models provide better robustness to distribution shifts, perhaps at the cost of reduced in-distribution performance?
- Especially in applications with very limited training data?
  e.g., dynamic MRI
- Can we use the "latest" generative models, namely score-based models, for patches?

Patch diffusion model: Simple version

Warm up:
simple, but less effective, approach:

- Fixed patch size
- Fixed patch grid
- No position information

(Fessler, Hu, Xu, BASP 2023 [48])



Patch-based score modeling

- Start with MRF formulation, aka *fields of experts* model [53–55] for image $\boldsymbol{x}$:

$$\mathrm{p}(\boldsymbol{x};\boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})} \mathrm{e}^{-\sum_c V_c(\boldsymbol{x};\boldsymbol{\theta})} = \frac{1}{Z(\boldsymbol{\theta})} \prod_c \mathrm{e}^{-V_c(\boldsymbol{x};\boldsymbol{\theta})}.$$

  - $\boldsymbol{\theta}$: parameter vector that describes the prior
  - V_c : *clique potential* for the cth image *patch*
  - $Z(\boldsymbol{\theta})$: (intractable) partition function
- Assume (temporarily) statistical spatial stationarity (image shift invariance):

$$V_c(\boldsymbol{x};\boldsymbol{\theta}) = V(\boldsymbol{G}_c \boldsymbol{x};\boldsymbol{\theta})$$

  - $\boldsymbol{G}_c$: wide binary matrix that grabs pixels of the cth patch from image $\boldsymbol{x}$
  - $V(\boldsymbol{v};\boldsymbol{\theta})$: common patch clique function

- Resulting log-prior:

$$\log \mathrm{p}(\boldsymbol{x}; \boldsymbol{\theta}) = -\log Z(\boldsymbol{\theta}) - \sum_c V(\boldsymbol{G}_c \boldsymbol{x}; \boldsymbol{\theta})$$

- Corresponding overall *image score function* arises from *patch score function*:

$$\boldsymbol{s}(\boldsymbol{x}; \boldsymbol{\theta}) \triangleq \nabla_{\boldsymbol{x}} \log \mathrm{p}(\boldsymbol{x}; \boldsymbol{\theta}) = \sum_c \boldsymbol{G}_c' \boldsymbol{s}_V(\boldsymbol{G}_c \boldsymbol{x}; \boldsymbol{\theta}), \qquad \boldsymbol{s}_V(\boldsymbol{v}; \boldsymbol{\theta}) \triangleq -\nabla_{\boldsymbol{v}} V(\boldsymbol{v}; \boldsymbol{\theta}).$$

- All we must learn is the patch score function $\boldsymbol{s}_V(\boldsymbol{v}; \boldsymbol{\theta}) : \mathbb{R}^n \mapsto \mathbb{R}^n$, *e.g.*, a UNet.
- For non-overlapping patches:

$$\underbrace{\left\| \boldsymbol{s}(\boldsymbol{x} + \boldsymbol{z}; \boldsymbol{\theta}) + \boldsymbol{z}/\sigma^2 \right\|_2^2}_{\text{image ``denoise''}} = \left\| \sum_c \boldsymbol{G}_c' \boldsymbol{s}_V(\boldsymbol{G}_c(\boldsymbol{x} + \boldsymbol{z}); \boldsymbol{\theta}) + \boldsymbol{z}/\sigma^2 \right\|_2^2$$

$$= \sum_c \underbrace{\left\| \boldsymbol{s}_V(\boldsymbol{x}_c + \boldsymbol{z}_c); \boldsymbol{\theta}) + \boldsymbol{z}_c/\sigma^2 \right\|_2^2}_{\text{patch ``denoise''}}, \quad \boldsymbol{z}_c \triangleq \boldsymbol{G}_c \boldsymbol{z}$$

Patch-based score learning (simple)

- For training image patches $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_T\}$, apply *denoising score matching* (DSM) of Vincent, 2011 [18], typically for a range of noise variances σ^2 [16]:

$$\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \frac{1}{T} \sum_{t=1}^{T} \mathsf{E}_{\sigma \sim p(\sigma)} \left[\sigma^2 \, \mathsf{E}_{\boldsymbol{z} \sim \mathcal{N}(0, \sigma^2 \boldsymbol{I}_n)} \left[\frac{1}{2} \left\| \boldsymbol{s}_V(\boldsymbol{v}_t + \boldsymbol{z}; \boldsymbol{\theta}, \sigma) + \frac{\boldsymbol{z}}{\sigma^2} \right\|_2^2 \right] \right].$$

- Final patch score model is $\boldsymbol{s}_V(\boldsymbol{v}; \hat{\boldsymbol{\theta}}, \sigma_{\min})$.
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$\Longrightarrow$ scales to large 2D images, 3D, 4D, etc.
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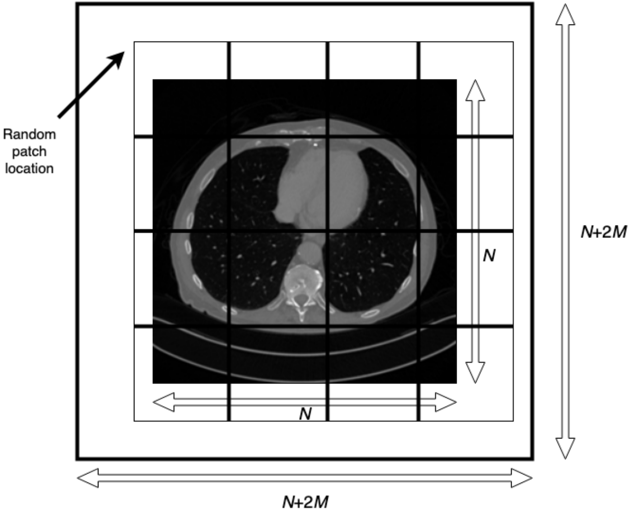
- Network input is just image patches, never the entire image
  $\Longrightarrow$ scales to large 2D images, 3D, 4D, etc.
- Drawbacks:
  - Visible patch boundaries
  - Fixed patch size slows learning
  - Suboptimal stationarity assumption (*cf.* vertebrae)

Improved patch modeling

- zero-pad image $\boldsymbol{x}$
- use multiple grid locations



Inspirations:

- Wavelet "cycle spinning" [49, 56–59]
- Wang, NeurIPS 2023 [60]

Probability model with padding & grids & positions

- $N_1 \times N_2$: original image size
- $P_1 \times P_2$: patch size
- $K_i \triangleq 1 + \lfloor N_i / P_i \rfloor,\ i = 1, 2$: # non-overlapping patches for original image
- $(N_1 + 2M_1) \times (N_2 + 2M_2)$: padded image size; $M_i \triangleq K_i P_i - N_i$
- Product probability model:

$$\mathrm{p}(\boldsymbol{x}) \triangleq \frac{1}{Z} \underbrace{\prod_{m=1}^{M_1 M_2}}_{\text{grid shifts}} \left(\underbrace{\mathrm{p}_{m,B}(\boldsymbol{x}_{m,B})}_{\text{border region}} \underbrace{\prod_{k=1}^{K_1 K_2} \mathrm{p}_{m,k}(\boldsymbol{x}_{m,k})}_{\text{patches}} \right) = \frac{1}{Z} \prod_{m=1}^{M_1 M_2} \prod_{k=1}^{K_1 K_2} \underbrace{\mathrm{e}^{-V(\boldsymbol{x}_{m,k};\, m, k)}}_{\text{position encoding}}$$

  - $\boldsymbol{x}_{m,B}$: border pixels for mth shift (all zero)
  - $\boldsymbol{x}_{m,k}$: kth patch for mth shift

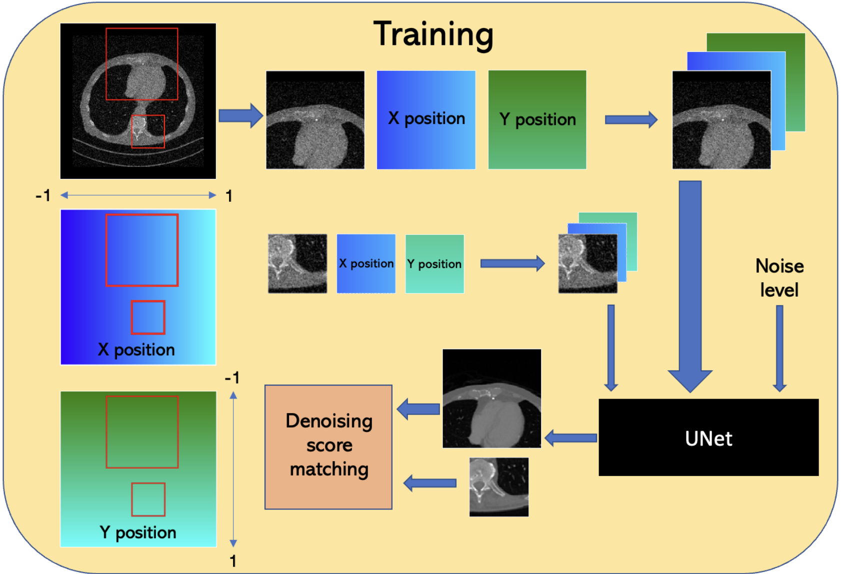
Probability model with padding & grids & positions

- $N_1 \times N_2$: original image size
- $P_1 \times P_2$: patch size
- $K_i \triangleq 1 + \lfloor N_i / P_i \rfloor,\ i = 1, 2$: # non-overlapping patches for original image
- $(N_1 + 2M_1) \times (N_2 + 2M_2)$: padded image size; $M_i \triangleq K_i P_i - N_i$
- Product probability model:

$$\mathrm{p}(\boldsymbol{x}) \triangleq \frac{1}{Z} \underbrace{\prod_{m=1}^{M_1 M_2}}_{\text{grid shifts}} \left(\underbrace{\mathrm{p}_{m,B}(\boldsymbol{x}_{m,B})}_{\text{border region}} \underbrace{\prod_{k=1}^{K_1 K_2} \mathrm{p}_{m,k}(\boldsymbol{x}_{m,k})}_{\text{patches}} \right) = \frac{1}{Z} \prod_{m=1}^{M_1 M_2} \prod_{k=1}^{K_1 K_2} \underbrace{\mathrm{e}^{-V(\boldsymbol{x}_{m,k};\, m, k)}}_{\text{position encoding}}$$

  - $\boldsymbol{x}_{m,B}$: border pixels for mth shift (all zero)
  - $\boldsymbol{x}_{m,k}$: kth patch for mth shift
- Learn position-dependent patch score function $\boldsymbol{s}(\boldsymbol{v}; \boldsymbol{\theta}, m, k) = -\nabla_{\boldsymbol{v}} V(\boldsymbol{v}; m, k)$

Patch Diffusion Inverse Solver (PaDIS): Training



NeurIPS 2024 [62]

Training images (CT)

AAPM 2016 CT challenge data [63];
10 3D volumes,
rescaled to 256^3

Example slices:

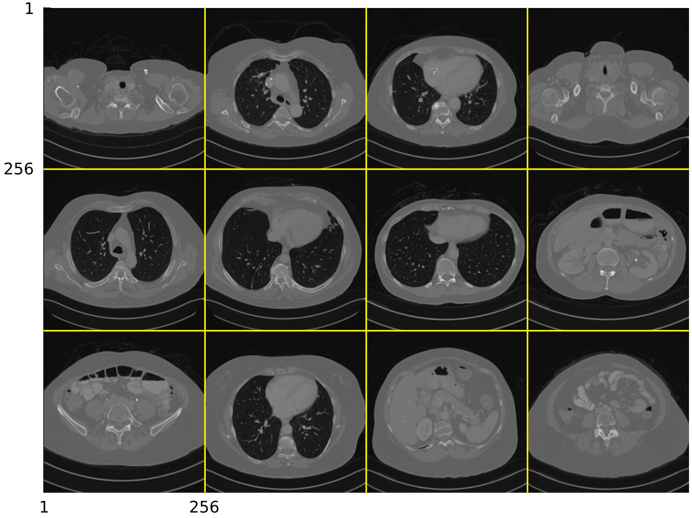
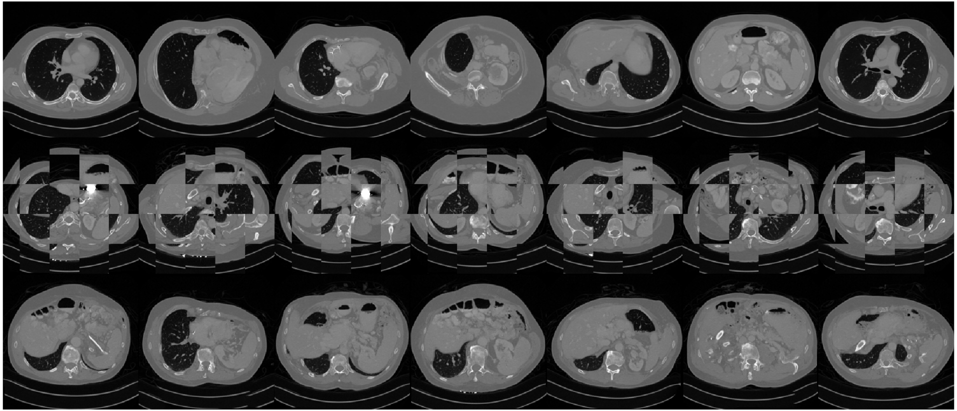


Image generation (unconditional sampling from prior)

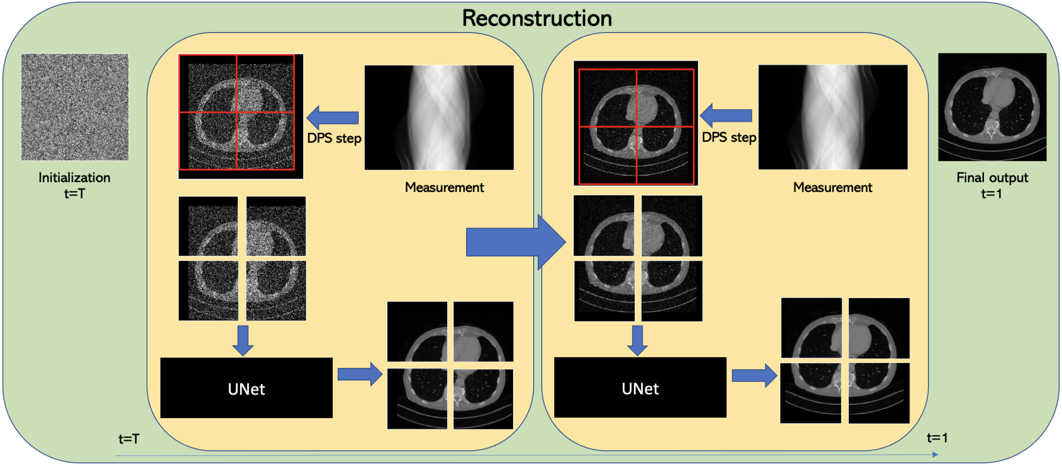


- Top: generation with a network trained on whole images (2D...)
- Middle: patch-only version of [60] (non-overlapping patches).
- Bottom: proposed PaDIS method.

Training time results

2 A40 GPUs using PyTorch and ADAM

- whole image model: 24 – 36 hours
- patch-based model: $\approx$ 12 hours



Diffusion posterior sampling (DPS) (Chung et al., ICLR 2023 [64]) with Langevin dynamics, modified to use patch score with random grid shifts.

PaDIS algorithm (modified from DPS)

Input: $\boldsymbol{y}$, $\boldsymbol{A}$, T, $\sigma_1 < \sigma_2 < \ldots < \sigma_T$, $\epsilon > 0$, $\{\zeta_t > 0\}$, P_1, P_2, M_1, M_2,
trained noise-conditional, position-encoded patch denoiser $\boldsymbol{d}(\cdot; \boldsymbol{\theta}_*, m, k, \sigma)$

Initialize random image $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{0}, \sigma_T^2 \boldsymbol{I})$

for $t = T : 1$ **do**

  Randomly select grid integer $m \in \{1, \ldots, M_1 M_2\}$

  for $k = 1 : (K_1 K_2)$ **do** (parallelizable)

    Extract patch $\boldsymbol{x}_{m,k}$

    Denoise patch: $\boldsymbol{d}_{m,k} \triangleq \boldsymbol{d}(\boldsymbol{x}_{m,k}; \boldsymbol{\theta}_*, m, k, \sigma_t)$

  end for

  Combine denoised patches to get denoised image $\boldsymbol{d}$

  Compute image score function: $\boldsymbol{s} = (\boldsymbol{d} - \boldsymbol{x}) / \sigma_t^2$

  Data term: $\boldsymbol{x} := \boldsymbol{x} - \zeta_t \nabla_{\boldsymbol{x}} \| \boldsymbol{A}\, \boldsymbol{d}(\boldsymbol{x}) - \boldsymbol{y} \|_2^2$

  Sample $\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{0}, \sigma_t^2 \boldsymbol{I})$

  Step size $\alpha_t \triangleq \epsilon\, \sigma_t^2$

  Langevin update: $\boldsymbol{x} := \boldsymbol{x} + \frac{\alpha_t}{2} \boldsymbol{s} + \sqrt{\alpha_t} \boldsymbol{z}$

end for

CT Experiments

Default setup:

- 9 of 10 volumes for training $\Longrightarrow$ 2304 slices
- 25 slices of 10th volume for testing
- 512 element parallel-beam CT detector
- $\boldsymbol{A}$ from Operator Discretization Library (ODL)
- 56×56 patch size
- U-Net of Karras 2022 [61]
- Step size $\zeta_t = \zeta / \|\boldsymbol{A}\boldsymbol{d}(\boldsymbol{x}_t) - \boldsymbol{y}\|_2$
- 1000 neural function evaluations (NFEs) [61]

Quantitative results on three different inverse problems

Method	CT, 20 Views		CT, 8 Views		Deblurring		Superresolution	
	PSNR↑	SSIM↑	PSNR↑	SSIM↑	PSNR↑	SSIM↑	PSNR↑	SSIM↑
Baseline	24.93	0.595	21.39	0.415	24.54	0.688	25.86	0.739
ADMM-TV	26.82	0.724	23.09	0.555	28.22	0.792	25.66	0.745
PnP-ADMM [65]	26.86	0.607	22.39	0.489	28.82	0.818	26.61	0.785
PnP-RED [66]	27.99	0.622	23.08	0.441	29.91	0.867	26.36	0.766
Whole image diffusion	32.84	0.835	25.74	0.706	30.19	0.853	29.17	0.827
Langevin dynamics [19]	33.03	0.846	27.03	0.689	30.60	0.867	26.83	0.744
Predictor-corrector [13]	32.35	0.820	23.65	0.546	28.42	0.724	26.97	0.685
VE-DDNM [67]	31.98	0.861	27.71	0.759	-	-	26.01	0.727
Patch Averaging [52]	33.35	0.850	28.43	0.765	29.41	0.847	27.67	0.802
Patch Stitching	32.87	0.837	26.71	0.710	29.69	0.849	27.50	0.780
PaDIS (Ours)	**33.57**	**0.854**	**29.48**	**0.767**	**30.80**	**0.870**	**29.47**	**0.846**

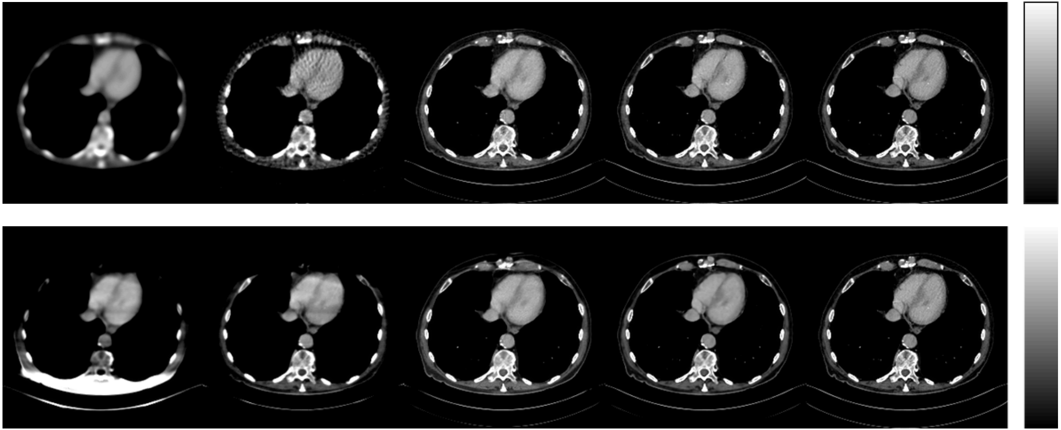
(Averages across all test images.)

More inverse problem experiments

Method	CT, 60 Views		CT, Fan Beam		Heavy Deblurring	
	PSNR↑	SSIM↑	PSNR↑	SSIM↑	PSNR↑	SSIM↑
Baseline	25.89	0.746	20.07	0.521	21.14	0.569
ADMM-TV	30.93	0.833	25.78	0.719	26.03	0.724
Whole image diffusion	35.83	0.894	26.89	0.835	28.35	0.808
PaDIS (Ours)	**39.28**	**0.941**	**29.91**	**0.932**	**28.91**	**0.818**

Example images

baseline FBP | ADMM-TV | whole image diffusion | PaDIS | ground truth



Top: 60 view CT
Bottom: fan-beam CT

≈ 400 HU window width

Effect of patch size P and positional encoding: CT

Patchsize

P	PSNR↑	SSIM↑
8	32.57	0.844
16	32.57	0.829
32	32.72	0.853
56	**33.57**	**0.854**
96	33.36	**0.854**
256	32.84	0.835

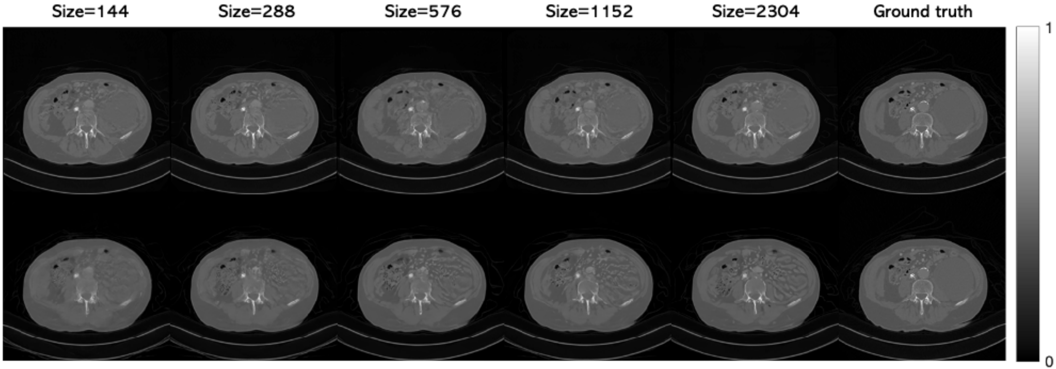
Positional encoding

	PSNR↑	SSIM↑
no position enc.	23.25	0.459
no position+init	24.51	0.518
with position	**33.57**	**0.854**

Effect of training dataset size on CT reconstruction

Dataset size	Patches 56×56		Whole image 256×256	
	PSNR↑	SSIM↑	PSNR↑	SSIM↑
144	32.28	0.841	29.12	0.804
288	32.43	0.837	31.09	0.829
576	33.03	0.846	31.81	0.835
1152	33.01	0.849	31.36	0.834
2304	**33.57**	0.854	32.84	0.835

20 view CT reconstruction: training dataset sizes



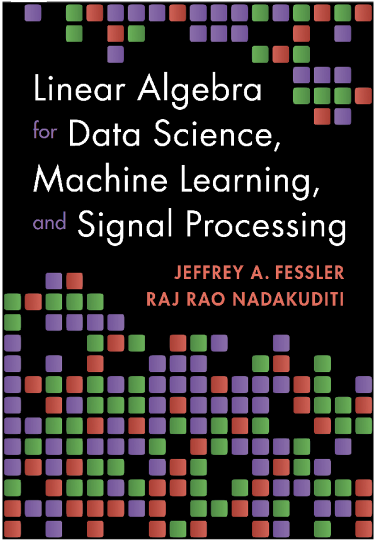
Top : PaDIS

Bottom : whole image diffusion model

Summary / future directions

- Generative models are promising for under-determined inverse problems
- Learning patch score models is feasible with denoising score matching
- For limited training data, patch-models can outperform whole-image models
- Integrate invariances: amplitude scale / rotation / flip / DC offset ...
- Explore trade-offs between generalizability and in-distribution performance
- Extend to 3D, 3D+Time, 3D+Multicontrast

Tutorial Julia code: `https://github.com/JeffFessler/ScoreMatching.jl`



- Online demos: `https://github.com/JeffFessler/book-la-demo`
- Topics include: low-rank matrix approximation, robust PCA, photometric stereo, video foreground/background separation, spectral clustering, matrix completion, ...
- Available from Cambridge Univ. Press

Resources

Talk and code available online at
`http://web.eecs.umich.edu/~fessler`

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