Learning Discrete Measurement Matrices and Algorithm Unfolding for Signal Recovery

Siyakhula - German Research Days at AIMS' 20-years Celebration, 2024

Peter Jung, Technical University Berlin
peter.jung@tu-berlin.de

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Inverse problems: given observation $\boldsymbol{y}$ and partially **known** forward operator $\boldsymbol{A}$:

$$\text{find} \quad \boldsymbol{x} \in \mathcal{X} \quad \text{s.t.} \quad \boldsymbol{A}(\boldsymbol{x}) \approx \boldsymbol{y}$$

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"Learn to sense and to recover"

$$\text{find} \quad (\boldsymbol{A}, \boldsymbol{Q}) \qquad \text{s.t.} \quad \mathbb{E}_{\boldsymbol{x} \sim \mathcal{X}} \, \textbf{loss}(\boldsymbol{x}, \boldsymbol{Q}(\boldsymbol{A}(\boldsymbol{x}))) \quad \text{"is small"}$$

Outline

Gradient-Based Learning of Discrete Structured Measurement Operators for Signal Recovery

Jonathan Sauder, Martin Genzel, and Peter Jung

***Abstract*—Countless signal processing applications include the reconstruction of signals from few indirect linear measurements. The design of effective measurement operators is typically constrained by the underlying hardware and physics, posing a challenging and often even discrete optimization task. While the potential of gradient-based learning via the unrolling of iterative recovery algorithms has been demonstrated, it has remained unclear how to leverage this technique when the set of admissible measurement operators is structured and discrete. We tackle this problem by combining unrolled optimization with Gumbel reparametrizations, which enable the computation of**

discrete subset—to improve the performance of downstream tasks poses great computational challenges. While it is often easy to create a suitable random mask, it is not obvious how to optimize the measurement matrix in a way that is both efficient and respects the feasibility constraints. Classical approaches commonly use discrete optimization to find such sets, as no gradients can be directly computed.

On the other hand, gradient-based optimization via back-propagation through massive nonlinear computational graphs

Problem Statement

- Recover $\boldsymbol{x} \in \mathcal{X} \subset \mathbb{R}^n$ from (noisy) linear measurements $\boldsymbol{y} = \boldsymbol{A}(\boldsymbol{x}) = \boldsymbol{\Phi}\boldsymbol{x} + \boldsymbol{e} \in \mathbb{R}^m$

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- $\boldsymbol{\Phi}$ lies in **finite set of admissible matrices** $\boldsymbol{\Phi}$ (determined by physics / detectors)
- $\boldsymbol{x}$ is recovered from $\boldsymbol{y}$ using parametrized recovery algorithm $f_{\boldsymbol{\theta},\boldsymbol{\Phi}} : \mathbb{R}^m \to \mathbb{R}^n$
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- $\boldsymbol{x} \to f_{\boldsymbol{\theta},\boldsymbol{\Phi}}(\boldsymbol{\Phi}\boldsymbol{x})$ can be understood as autoencoder
- find good and **admissible** $\boldsymbol{\Phi} \in \boldsymbol{\mathit{\Phi}}$ and algorithm parameters $\boldsymbol{\theta}$

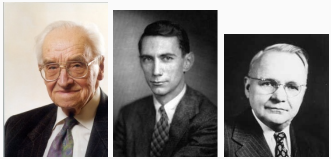
$$\min_{\boldsymbol{\Phi}\in\boldsymbol{\mathit{\Phi}},\boldsymbol{\theta}} \mathbb{E}_{\boldsymbol{x}\sim\mathcal{X}} \left[\mathbf{loss}(f_{\boldsymbol{\theta},\boldsymbol{\Phi}}(\boldsymbol{\Phi}\boldsymbol{x}), \boldsymbol{x}) \right]$$

data-driven via "training"

prototypical playground is **"compressed sensing"** $\Leftrightarrow$ recovering sparse $\boldsymbol{x}$ from $\boldsymbol{y} = \boldsymbol{\Phi}\boldsymbol{x} + \boldsymbol{e}$

classical sampling/scanning *"…if you sample densely enough, you can perfectly reconstruct the original analog data…"*

- ☺ good, if signals "fill up" a subspace (linear structure)
- ☹ wasteful for compressible signals (non–linear structure)



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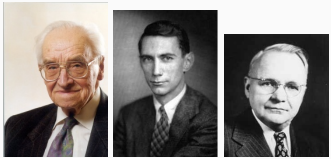

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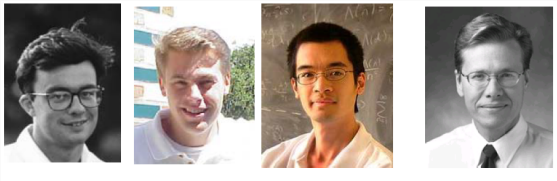

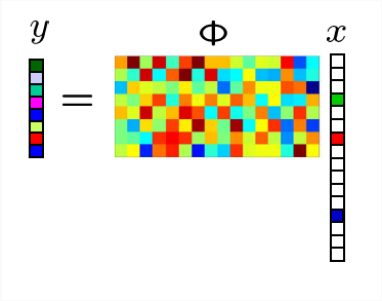

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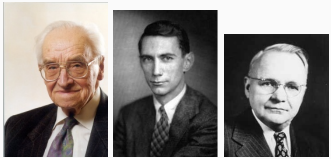

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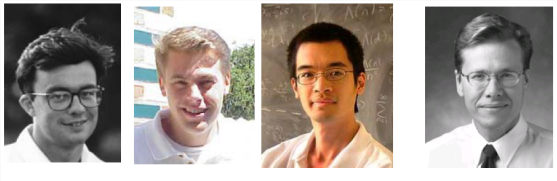

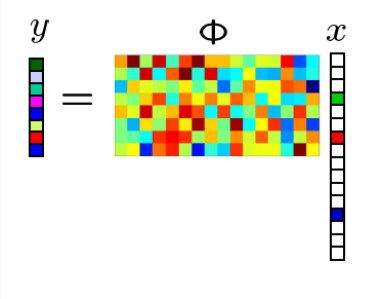

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- ☺ Well-investigated, theoretical bounds, algorithms

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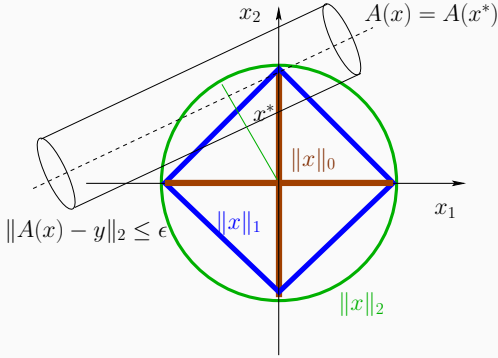
Convex recovery approach with guarantees

$$x^\sharp = \arg\min \|z\|_1 \quad \text{s.t.} \quad \|\Phi z - y\| \leq \epsilon$$



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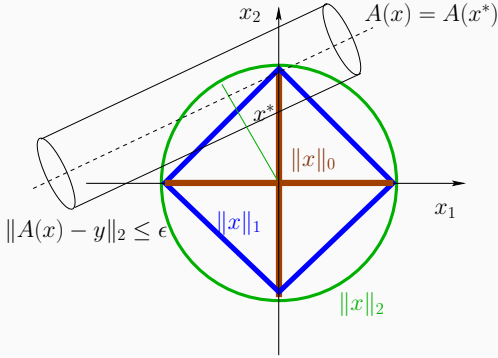
holds for all $y = \Phi x + e$ with $\|e\| \leq \epsilon$.



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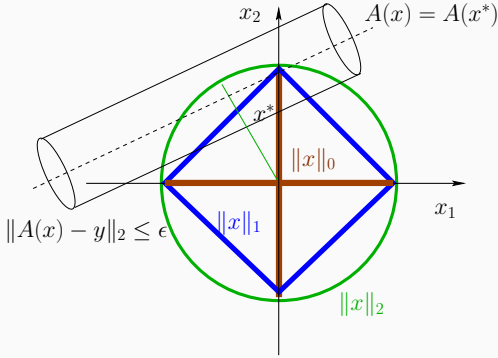

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- ☺ Non-negativity & "biased" measurements are helpful, example later

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in "machine learning" terminology:

$$\min_{p,\boldsymbol{\theta}} \mathbb{E}_{\boldsymbol{x},\mathbf{\Phi}\sim p}[\mathbf{loss}(f_{\boldsymbol{\theta},\mathbf{\Phi}}(\mathbf{\Phi}x), x)]$$

two techniques: **Gumbel reparametrizations** and **algorithm unfolding**

Gradient-based Learning of Discrete Measurement Matrices

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1. Gradient descent on p but estimate $\nabla_p \mathbb{E}_{\mathbf{\Phi}\sim p} f(\mathbf{\Phi})$ via **sampling**
2. perform sampling in a way that allows backprop - **Gumbel reparametrization**

- Consider computational graph with a *random node* v taking the values in $[a] := \{1, \dots, a\}$.
- inputs to node v are unnormalized log-probabilities $\boldsymbol{\varphi} = (\varphi_1 \ \dots, \varphi_a) \in \mathbb{R}^a$

$$\mathbb{P}(v = i) = \frac{\exp(\varphi_i)}{\sum_{j=1}^{a} \exp(\varphi_j)} = \mathsf{softmax}(\boldsymbol{\varphi})_i, \quad i = 1, \dots, a$$

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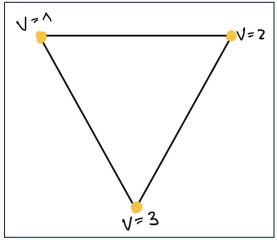
- efficiently sample from v by using [Gumbel 1954]

$$\boldsymbol{v} = \mathsf{one\_hot}(\arg\max_i [\varphi_i + g_i])$$

where $g_i = -\log(-\log(u_i))$ with $u_1, \dots, u_a \sim_{\text{iid}} \mathsf{unif}([0, 1])$



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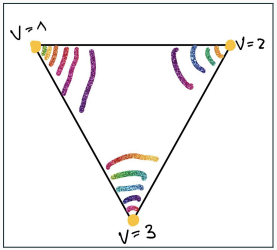
☺ **Gumbel-softmax** [Jang et al. 2016; Maddison et al. 2016]
replace $\arg\max$ in backward pass with softmax with temperature τ:

$$v_i = \frac{\exp((g_i + \varphi_i)/\tau)}{\sum_{j=1}^{a} \exp((g_j + \varphi_j)/\tau)} = \text{softmax}((\boldsymbol{\varphi} + \boldsymbol{g})/\tau)_i$$

- As $\tau \to 0$, softmax approaches $\arg\max$



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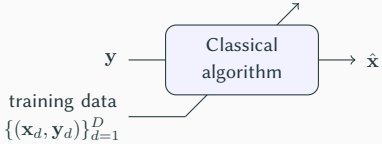
ok, now we also need a "trainable" recovery algorithm ...

Algorithm Unfolding



Computational graph of many iterative algorithms can be viewed as neural networks…

- consider for example:

$$\min_{x} \|\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{x}\|_2^2 + \lambda g(\boldsymbol{x})$$

and use proximal (Landweber) iterations:

$$\hat{\boldsymbol{x}}^{(t+1)} = \text{prox}_{\lambda g}\Big(\hat{\boldsymbol{x}}^{(t)} + \gamma \nabla\big(\|\boldsymbol{y} - \boldsymbol{\Phi}\hat{\boldsymbol{x}}^{(t)}\|_2^2\big)\Big),$$

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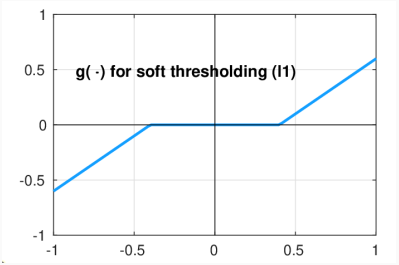
- $g(\boldsymbol{x}) = \|\boldsymbol{x}\|_1 \Rightarrow$ element-wise soft-thresholding, known as *Iterative Shrinkage and Thresholding Algorithm* [Daubechies et al., 2004]

(ISTA) $$\hat{\boldsymbol{x}}^{(t+1)} = \eta_{\frac{\lambda}{L}}\Big(\hat{\boldsymbol{x}}^{(t)} + \gamma\boldsymbol{\Phi}^*(\boldsymbol{\Phi}\hat{\boldsymbol{x}}^{(t)} - \boldsymbol{y})\Big)$$



Unfolding iterations into network $f_{\boldsymbol{\theta},\boldsymbol{\Phi}}$, several proposals [Gregor&LeCun 2010, Liu 2019, Chen 2018,...]:

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- supervised training on $\mathcal{X}$ with $\mathbb{E}_{\boldsymbol{x}\sim\mathcal{X},\boldsymbol{e}}$ **loss**$(f_{\boldsymbol{\theta},\boldsymbol{\Phi}}(\boldsymbol{\Phi}\boldsymbol{x}+\boldsymbol{e}),\boldsymbol{x})$, unsupervised is possible as well
- $\mathcal{X}$ = bounded s-sparse vectors and cross-coherence $\mu := \mu(\boldsymbol{B},\boldsymbol{\Phi})$

Theorem: [Liu et al., 2019 ; Hauffen, PJ, Mücke 2022]

For any $\boldsymbol{x} \in \mathcal{X}$ with $s < (\mu^{-1}+1)/2$, $\|\boldsymbol{e}\|_2 \leq \epsilon$ and $\alpha^{(k)} \gtrsim \mu + \epsilon$ **ALISTA** yields:

$$\|\boldsymbol{x}^{(k)} - \boldsymbol{x}\|_2 \lesssim c^k s + \left(1 + kc^k\right)\|\boldsymbol{e}\|_2$$

for $c = c(\{\alpha_{k'}\}_{k'=1}^k) < 1$ and constants depend on $\mathcal{X}$ and $\{\alpha_{k'}\}_{k'=1}^k$.

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- *neurally augmented ALISTA* (NA-ALISTA) [Behrens, Sauder, PJ 2020]:

$$\boldsymbol{x}^{(k+1)} = \eta_{\alpha(r^{(k)}, u^{(k)})}\left(\boldsymbol{x}^{(k)} - \gamma(r^{(k)}, u^{(k)})\left[\boldsymbol{B}^*\left(\boldsymbol{\Phi}\boldsymbol{x}^{(k)} - \boldsymbol{y}\right)\right]\right)$$

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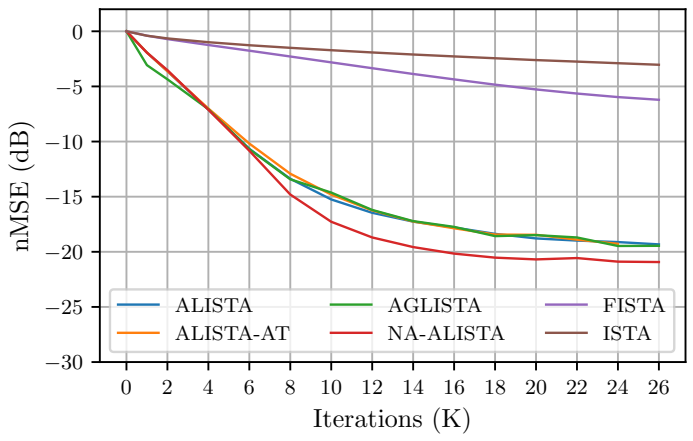
Significantly reduces number of iterations required! Enabling real-time applications



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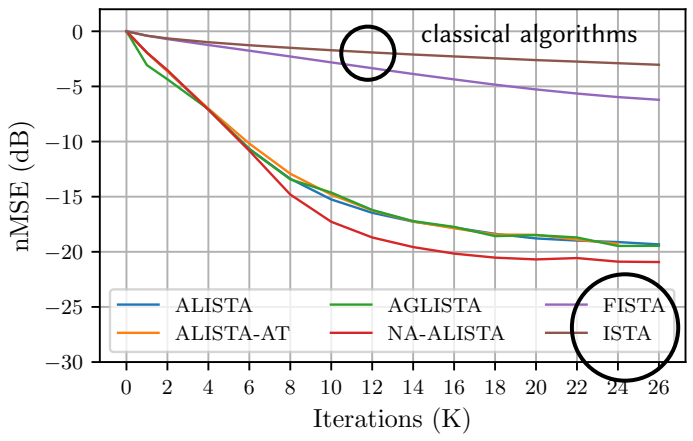

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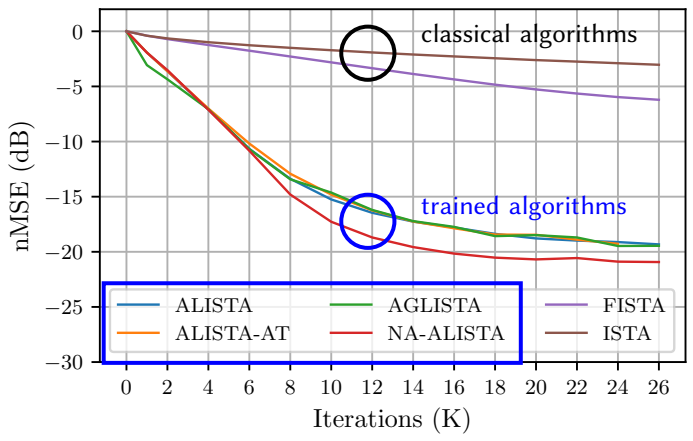
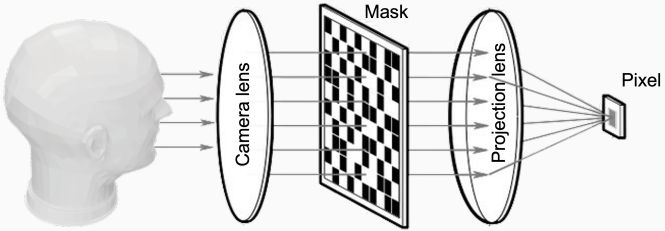


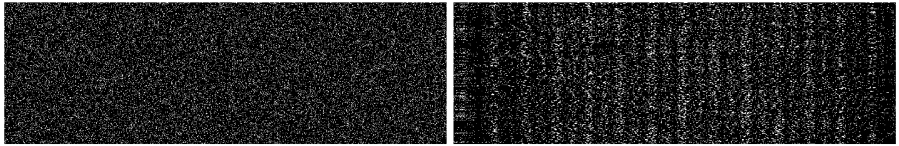
Application 1: Learning Masks for Single-Pixel Imaging



[adapted from [Bacca et al. 2019]]

- $\mathcal{X}$ =MNIST ($n = 28^2 = 784$)
- $\boldsymbol{\Phi}$ is the set of **binary matrices** with $k_i = 32$ ones per row i ("on"-pixels per mask)
- $f_{\boldsymbol{\theta},\boldsymbol{\Phi}}$ is NA-ALISTA with $T = 20$ layers/iterations
- $\mathcal{L}(\hat{x}, x) = \|\hat{x} - x\|_2^2$

(a) Random Masks (b) Learned Masks

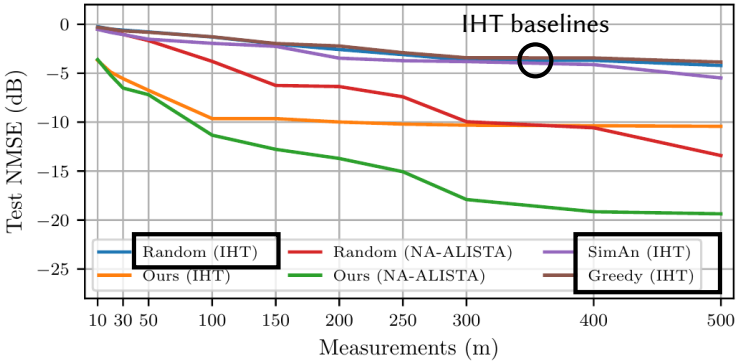


(c) Random Φ (d) Learned Φ

(e) Reconstructed (random Φ) (f) Reconstructed (learned Φ)

baseline: Iterative Hard-thresholding (IHT) $\boldsymbol{x}^{(k+1)} = H_s\left(\boldsymbol{x}^{(k)} - \boldsymbol{\Phi}^*\left(\boldsymbol{\Phi}\boldsymbol{x}^{(k)} - \boldsymbol{y}\right)\right)$

- $n = 28^2 = 784$ ($\mathcal{X}$=MNIST)
- random $I \subset \mathcal{I} = [m] \times [n]$
- swap a random $1 \Leftrightarrow 0$
- accept if loss L decreases
- **Greedy:** not accept if L increase
- **SimAn:** accept if $\exp[(L - L')/\tau] \leq u \sim U(0,1)$ and $\tau \to 0$ with training



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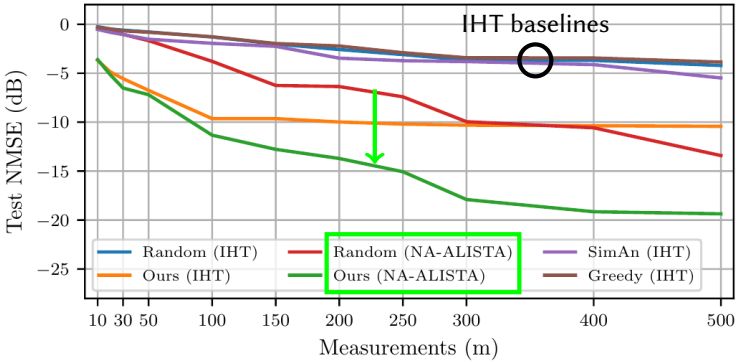

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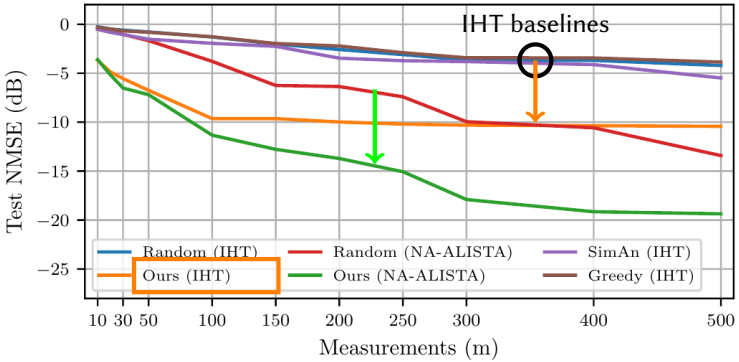
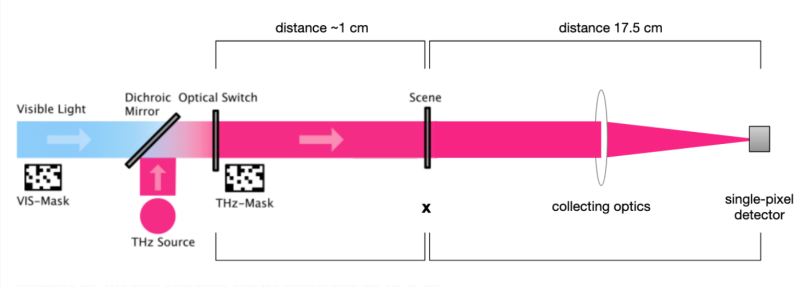
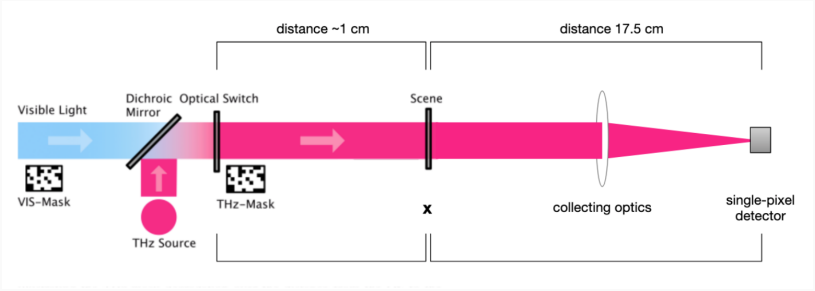


☺ **Improvements for IHT while trained with NA-ALISTA ⇒ due to Φ**



Terahertz SPI [Augustin, PJ, Frohmann, Hübers, 2019] - image: [Reiche, PJ 2020]

- wavelength is in order of pixel size, diffraction degrades image quality ⇒ use super-pixels!



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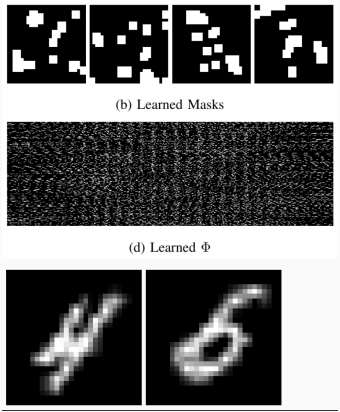

- wavelength is in order of pixel size, diffraction degrades image quality ⇒ use super-pixels!
- sample binary masks with d **ones forming super-pixels of size** Δ

Application 2: Learning Pooling Matrices for Group Testing

- **Non-adaptive viral testing of n individuals with minimal amount of m qPCR-tests**
- $s \ll n$ individuals are positive, i.e., vector of viral loads $\boldsymbol{x} = (x_1, \ldots, x_n)$ **is sparse**

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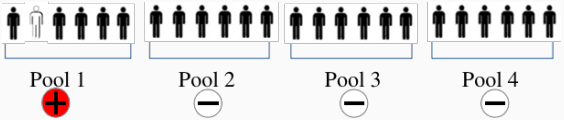

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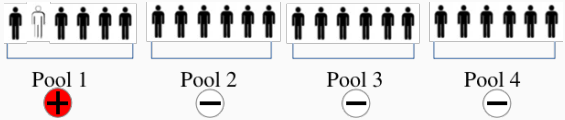

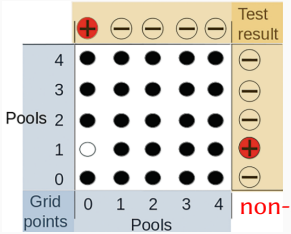

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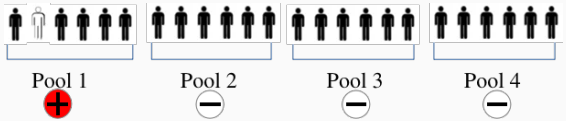

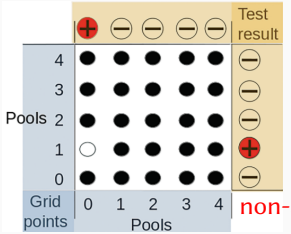

non-adaptive testing

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- binary pooling matrix $\boldsymbol{\Phi} \in \{0,1\}^{m \times n}$ has k non-zeros per row (pool size)
- pooled measurements of viral loads are $\boldsymbol{y} = \boldsymbol{\Phi x} + \boldsymbol{e}$ with sparse $\boldsymbol{x} \geq 0$

- qPCR modeling is complicated and involves multiplicative noise, yielding heavy-tailed models
- **non-negative least absolute deviations** (NNLAD) is a compressed sensing algorithm

$$\hat{\boldsymbol{x}} = \arg\min_{\boldsymbol{x} \geq 0} \|\boldsymbol{\Phi}\boldsymbol{x} - \boldsymbol{y}\|_1$$

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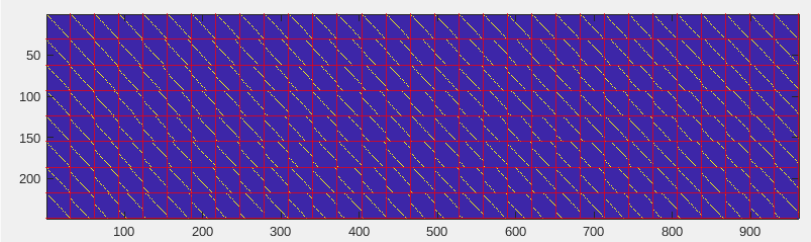
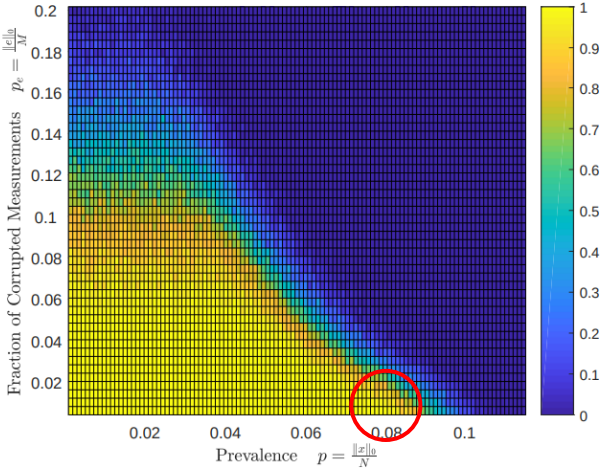


Example: disjunct matrix $\boldsymbol{\Phi} \in \{0,1\}^{248\times 961}$ with $k = 31$ and has NSP for $s \leq 7$ (LDPC/Array code) [Lofti&Vidyasagar, 2020]

robust against corrupted tests (sparse noise) and **empirical success up to** $s \lesssim 70$ **!!**



Learning pooling matrices (k ones per row) and tuning viral load recovery

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- slow convergence (not relevant for testing)
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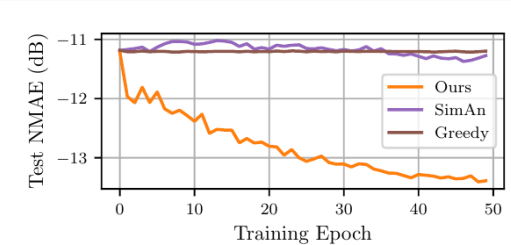

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☺ examples in single-pixel/detector imaging and pooling

Thank you!

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