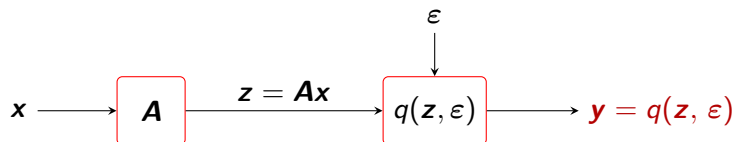


Bayes-optimal Estimation in Generalized Linear Models

Ramji Venkataramanan, University of Cambridge
(Joint work with Pablo Pascual Cobo and Kuan Hsieh)

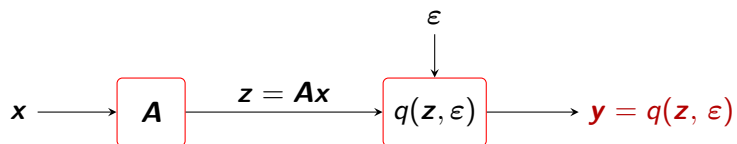
Generalized Linear Models



GOAL:

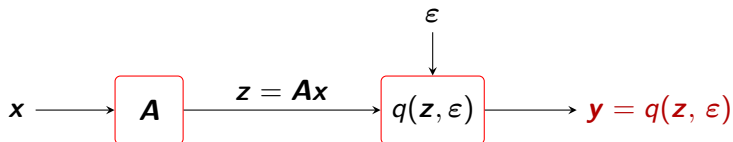
- ▶ Estimate signal $\mathbf{x} \in \mathbb{R}^n$ from observations $\mathbf{y} \equiv (y_1, \dots, y_m)$
- ▶ Known sensing matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ and output function q

Examples



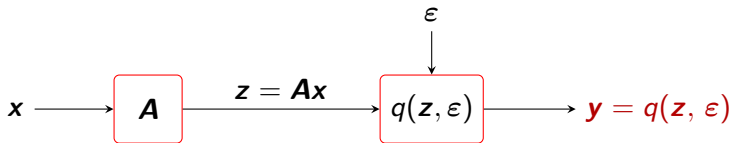
- ▶ Linear model $y = Ax + \epsilon$

Examples

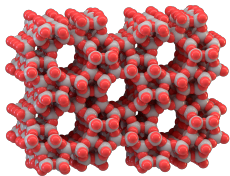


- ▶ Linear model $\mathbf{y} = \mathbf{A}\mathbf{x} + \epsilon$
- ▶ 1-bit compressed sensing $\mathbf{y} = \text{sign}(\mathbf{A}\mathbf{x} + \epsilon)$

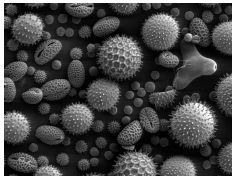
Examples



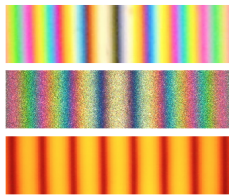
- ▶ Linear model $\mathbf{y} = \mathbf{A}\mathbf{x} + \epsilon$
- ▶ 1-bit compressed sensing $\mathbf{y} = \text{sign}(\mathbf{A}\mathbf{x} + \epsilon)$
- ▶ Phase retrieval $\mathbf{y} = |\mathbf{A}\mathbf{x}|^2 + \epsilon$



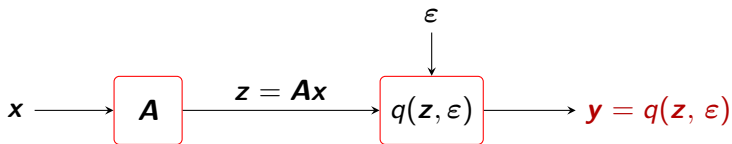
X-ray crystallography



Microscopy



Interferometry

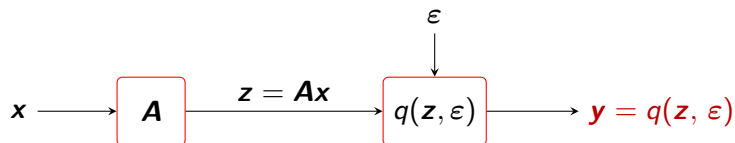


$$\mathbf{A} = \begin{bmatrix} \leftarrow & \mathbf{a}_1 & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{a}_m & \rightarrow \end{bmatrix} \in \mathbb{R}^{m \times n}$$

High-dimensional regime

$$\frac{m}{n} \rightarrow \delta \text{ as } m, n \rightarrow \infty$$

Bayesian setting



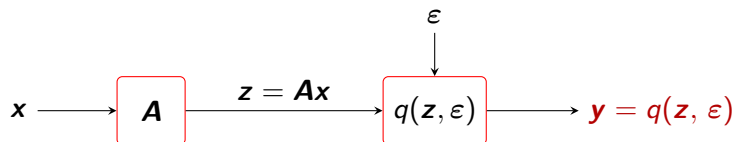
Suppose:

- ▶ $\mathbf{x} \sim P_{\mathbf{X}}$ and $\epsilon \sim P_{\epsilon}$
- ▶ \mathbf{A} also generated from known distribution

Bayes-optimal estimator that minimizes MSE: $\mathbb{E}\{\mathbf{x} \mid \mathbf{A}, \mathbf{y}\}$

$$\text{MMSE}_n := \frac{1}{n} \mathbb{E}\{\|\mathbf{x} - \mathbb{E}\{\mathbf{x} \mid \mathbf{A}, \mathbf{y}\}\|^2\}.$$

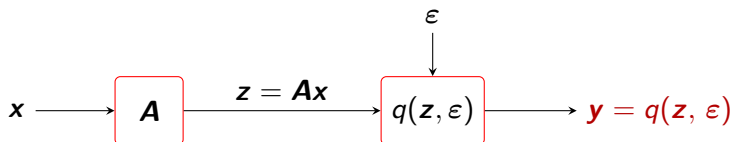
Two natural questions



$$\text{MMSE}_n := \frac{1}{n} \mathbb{E} \{ \|\mathbf{x} - \mathbb{E}\{\mathbf{x} \mid \mathbf{A}, \mathbf{y}\}\|^2 \}.$$

1. What is $\lim_{n \rightarrow \infty} \text{MMSE}_n$? (for a fixed $\delta = \lim \frac{m}{n}$)

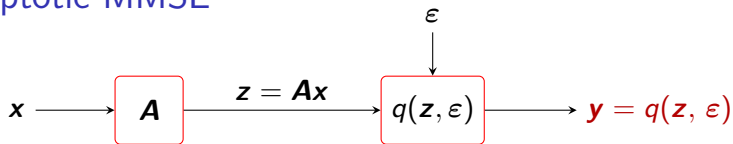
Two natural questions



$$\text{MMSE}_n := \frac{1}{n} \mathbb{E} \{ \|\mathbf{x} - \mathbb{E}\{\mathbf{x} \mid \mathbf{A}, \mathbf{y}\}\|^2 \}.$$

1. What is $\lim_{n \rightarrow \infty} \text{MMSE}_n$? (for a fixed $\delta = \lim \frac{m}{n}$)
2. How can we design **efficient** estimators whose error approaches $\lim \text{MMSE}_n$?

Asymptotic MMSE



- ▶ For iid Gaussian \mathbf{A} with $A_{ij} \sim \mathcal{N}(0, \frac{1}{n})$
- ▶ Signal \mathbf{x} iid $\sim P_X$ and noise ϵ iid $\sim P_\epsilon$

[Barbier et al. '19]: Formula for asymptotic MMSE in terms of a scalar **potential function** $U(x; \delta)$

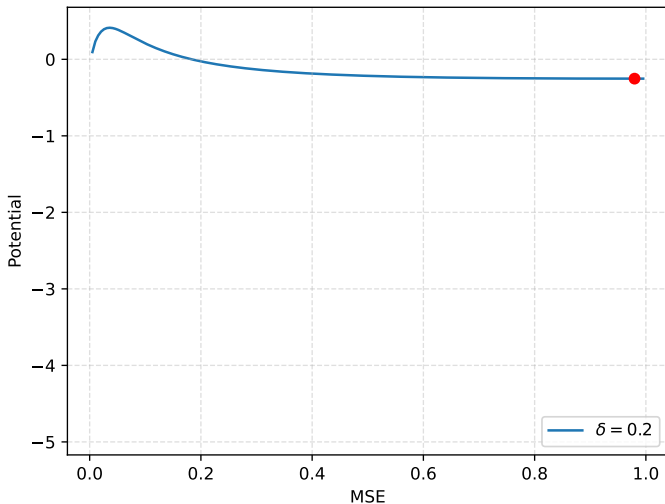
$$\lim_{n \rightarrow \infty} \text{MMSE}_n = \arg \min_{x \in [0, \text{Var}(X)]} U(x; \delta)$$

$$\lim_{n \rightarrow \infty} \frac{1}{n} I(\mathbf{X}; \mathbf{Y}) = \min_{x \in [0, \text{Var}(X)]} a U(x; \delta) + b$$

Example: Phase Retrieval

$$\mathbf{y} = |\mathbf{Ax}|^2 \quad \text{Prior } P_X(-a) = 0.4, P_X(a) = 0.6$$

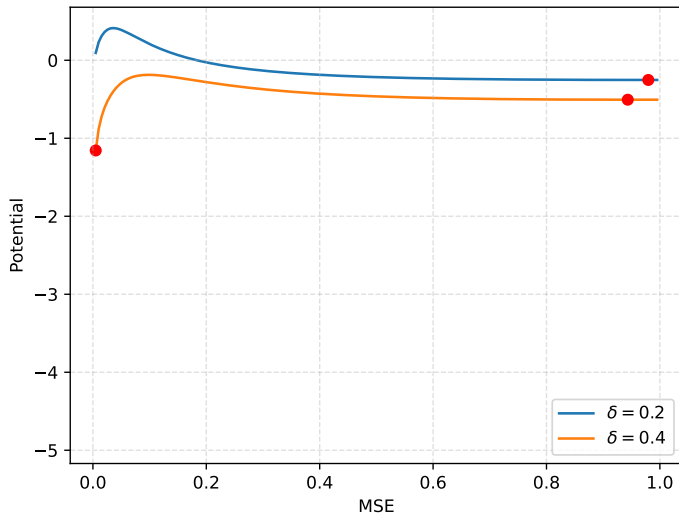
$U(x; \delta)$ vs x



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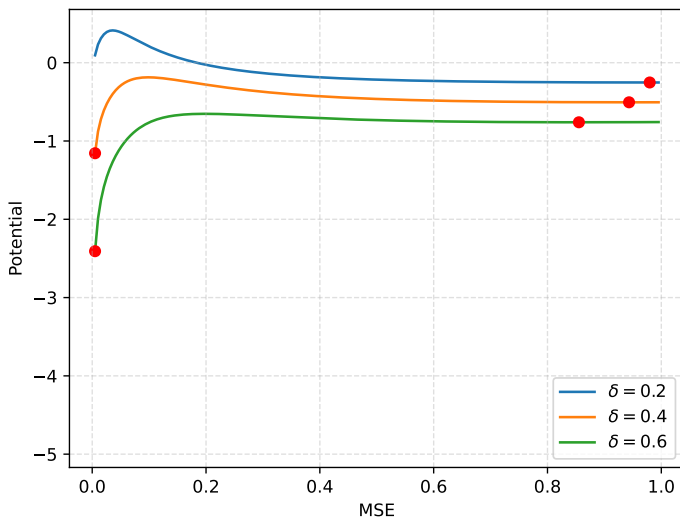
$U(x; \delta)$ vs x



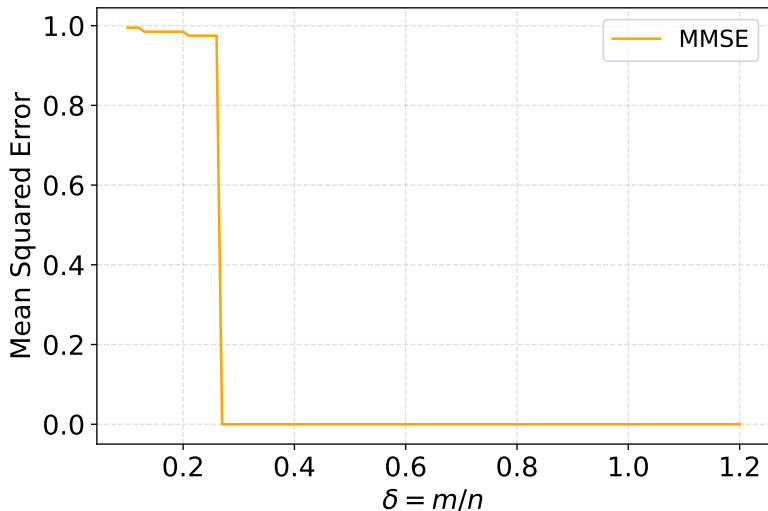
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$U(x; \delta)$ vs x



MMSE: Phase retrieval



Can we achieve this with efficient estimators?

Estimators

- ▶ Convex relaxations
- ▶ Iterative algorithms for non-convex objectives:
Alternating minimization, gradient descent, ...
- ▶ Spectral methods

Phase retrieval: [Netrapalli et al. '13], [Candes et al. '13], [Luo et al. '19], [Mondelli & Montanari '19], ...

1-bit CS: [Plan & Vershynin '13], [Jacques et al. '13], ...

Estimators

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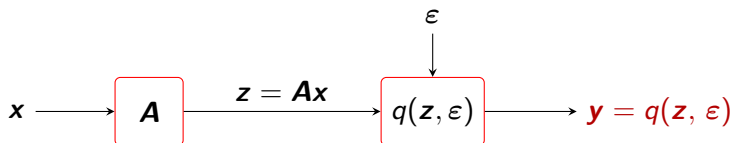
Generic techniques: can incorporate certain constraints like sparsity

But not well-equipped to exploit specific structural info about signal, e.g., known prior

Phase retrieval: [Netrapalli et al. '13], [Candes et al. '13], [Luo et al. '19], [Mondelli & Montanari '19], ...

1-bit CS: [Plan & Vershynin '13], [Jacques et al. '13], ...

Approximate Message Passing



Estimator based on **AMP**

- ▶ Can be tailored to take advantage of prior info about signal
- ▶ Rigorous performance characterization via **state evolution**
Allows us to precisely compute asymptotic MSE

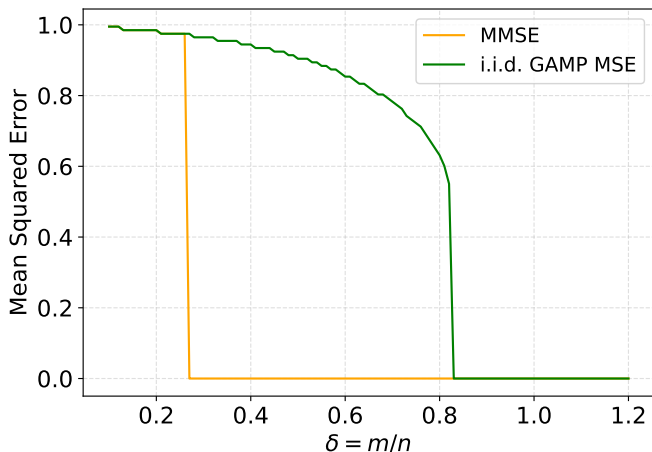
GAMP [Rangan '11]: for GLMs with i.i.d. Gaussian A

– Conjectured to be optimal among poly-time estimators

AMP vs MMSE estimator

Phase retrieval with i.i.d. Gaussian \mathbf{A}

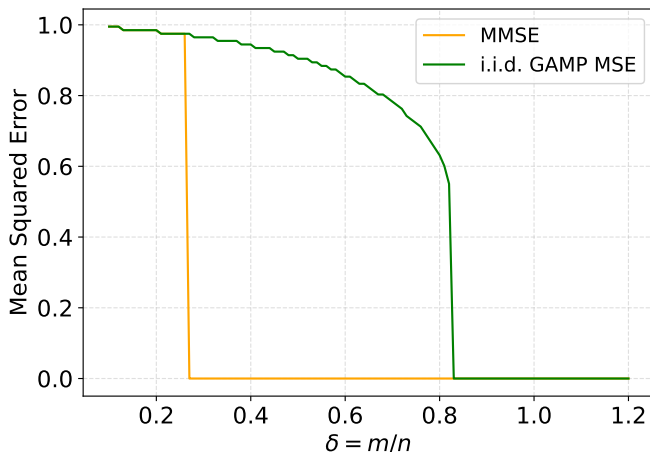
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AMP vs MMSE estimator

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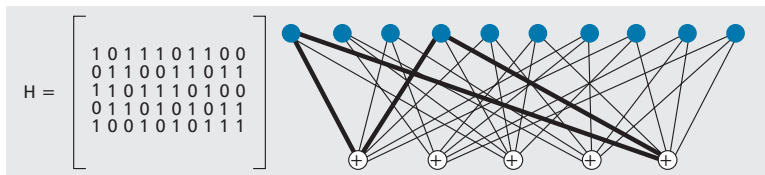
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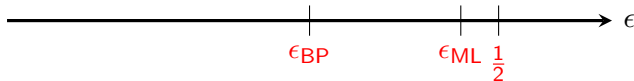
This talk: How to close this gap?

Parallel with coding theory

Consider a rate $R = \frac{1}{2}$ **regular** LDPC code. E.g.,



Used over channel with erasure probability ϵ



ϵ_{BP} : Threshold with belief propagation decoding

ϵ_{ML} : Threshold with optimal (ML) decoding

Figure from Costello et al. *Spatially coupled sparse codes on graphs: theory and practice*, 2014

Closing the gap: Can make ϵ_{BP} approach ϵ_{ML} with **spatially coupled code** [Kudekar et al. '14]

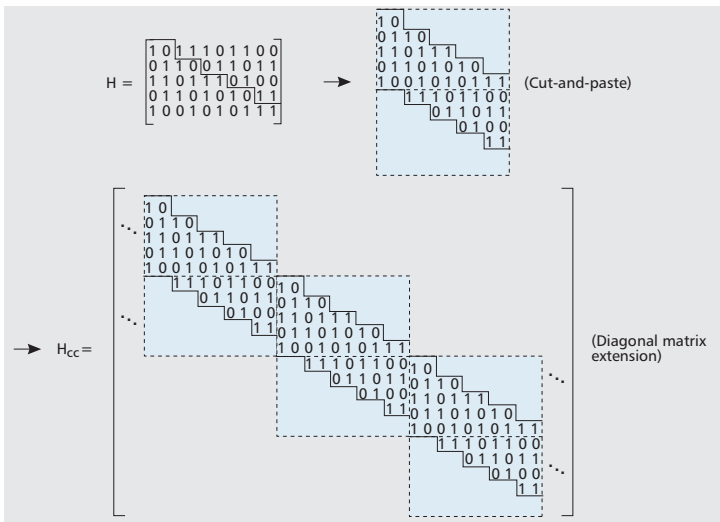


Figure from Costello et al. *Spatially coupled sparse codes on graphs: theory and practice*, 2014

LDPC codes

Rate R

Regular parity check matrix

BP decoder

Density evolution

GLM

Sampling ratio δ

iid Gaussian sensing matrix

AMP estimator

State evolution

LDPC codes

Rate R

Regular parity check matrix

BP decoder

Density evolution

ϵ_{BP} , ϵ_{ML}

Spatially coupled code

GLM

Sampling ratio δ

iid Gaussian sensing matrix

AMP estimator

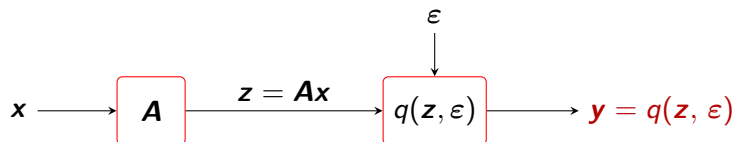
State evolution

δ_{AMP} , δ_{MMSE}

Spatially coupled sensing matrix

Compressed sensing: [Kudekar, Pfister '10], [Donoho, Javanmard, Montanari '13] ...

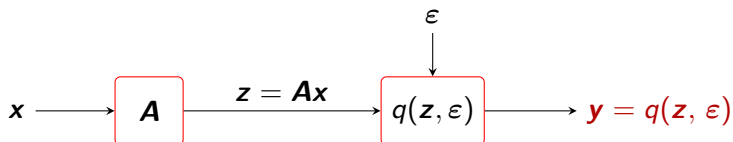
i.i.d. Gaussian GAMP



Iteratively produces estimates $\mathbf{x}(t)$ and $\mathbf{z}(t)$ for $t \geq 0$ via:

$$g_{\text{in}}(\cdot; t) : \mathbb{R} \rightarrow \mathbb{R}, \quad g_{\text{out}}(\cdot, y; t) : \mathbb{R}^2 \rightarrow \mathbb{R}$$

i.i.d. Gaussian GAMP



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$$\mathbf{x}(t+1) = g_{\text{in}}(\mathbf{x}(t); t) + \alpha^{\mathbf{x}}(t+1) \mathbf{A}^{\text{T}} g_{\text{out}}(\mathbf{z}(t), \mathbf{y}; t)$$

$$\mathbf{z}(t+1) = \mathbf{A} g_{\text{in}}(\mathbf{x}(t+1); t+1) - \alpha^{\mathbf{z}}(t+1) g_{\text{out}}(\mathbf{z}(t), \mathbf{y}; t)$$

i.i.d. Gaussian GAMP

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- ▶ \mathbf{g}_{in} and \mathbf{g}_{out} applied row-wise
- ▶ $\mathbf{g}_{\text{in}}, \mathbf{g}_{\text{out}}$ Lipschitz, allow us to tailor the algorithm

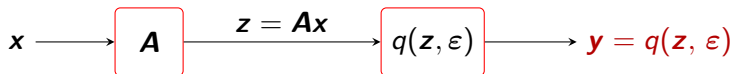
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- ▶ \mathbf{g}_{in} and \mathbf{g}_{out} applied row-wise
- ▶ $\mathbf{g}_{\text{in}}, \mathbf{g}_{\text{out}}$ Lipschitz, allow us to tailor the algorithm
- ▶ Initialized with \mathbf{x}^0 and $\mathbf{z}(0) = \mathbf{A}\mathbf{x}^0$
- ▶ Coefficients $\alpha^{\mathbf{x}}(t)$ and $\alpha^{\mathbf{z}}(t)$ defined in terms of \mathbf{g}_{in}' and \mathbf{g}_{out}'

Asymptotics of i.i.d Gaussian GAMP

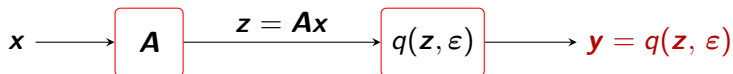


$$\mathbf{x}(t+1) = \mathbf{g}_{\text{in}}(\mathbf{x}(t); t) + \alpha^{\mathbf{x}}(t+1)\mathbf{A}^{\text{T}}\mathbf{g}_{\text{out}}(\mathbf{z}(t), \mathbf{y}; t)$$

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Suppose empirical distribution of \mathbf{x} converges to law of $X \sim P_X$.
Then as $n \rightarrow \infty$:

Asymptotics of i.i.d Gaussian GAMP



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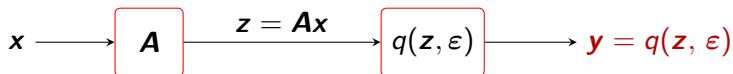
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Then as $n \rightarrow \infty$:

The empirical distribution of $(\mathbf{x}, \mathbf{x}(t))$ converges to the law of

$$[X, \mu(t) X + W(t)], \quad \text{where } W(t) \sim \text{N}(0, \tau(t))$$

Asymptotics of i.i.d Gaussian GAMP



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Suppose empirical distribution of \mathbf{x} converges to law of $X \sim P_X$.
Then as $n \rightarrow \infty$:

The empirical distribution of $(\mathbf{z}, \mathbf{z}(t))$ converges to the law of

$$[\mathbf{Z}, \mathbf{Z}(t)] \sim \mathbf{N}(0, \Lambda(t))$$

State Evolution

The empirical distribution of $(\mathbf{x}, \mathbf{x}(t))$ converges to the law of

$$[X, \mu(t)X + W(t)], \quad \text{where } W(t) \sim N(0, \tau(t))$$

The empirical distribution of $(\mathbf{z}, \mathbf{z}(t))$ converges to the law of

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$\mu(t), \tau(t), \Lambda(t)$ computed via **state evolution** recursion:

$$[\mu(t), \tau(t), \Lambda(t)] \longrightarrow [\mu(t+1), \tau(t+1), \Lambda(t+1)]$$

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$$[\mu(t), \tau(t), \Lambda(t)] \longrightarrow [\mu(t+1), \tau(t+1), \Lambda(t+1)]$$

- ▶ State evolution depends on g_{in} and g_{out}
- ▶ Analogous to density evolution for LDPC codes

Bayes GAMP

Asymptotic MSE: For $t \geq 1$,

$$\lim_{n \rightarrow \infty} \frac{1}{n} \|\mathbf{x} - \mathbf{g}_{\text{in}}(\mathbf{x}(t))\|^2 = \mathbb{E}\{[X - \mathbf{g}_{\text{in}}(\mu(t)X + W(t))]^2\}$$

Bayes GAMP

Asymptotic MSE: For $t \geq 1$,

$$\lim_{n \rightarrow \infty} \frac{1}{n} \|\mathbf{x} - g_{\text{in}}(\mathbf{x}(t))\|^2 = \mathbb{E}\{[X - g_{\text{in}}(\mu(t)X + W(t))]^2\}$$

- ▶ Bayes-optimal choice of g_{in} :

$$g_{\text{in}}^*(X(t)) = \mathbb{E}[X \mid \mu(t)X + W(t) = X(t)]$$

$g_{\text{in}}^*(\mathbf{x}(t))$ is the MMSE estimate of \mathbf{x} given $\mathbf{x}(t)$

- ▶ Can also determine Bayes-optimal g_{out}^*

Fixed points of Bayes GAMP

$$\lim_{n \rightarrow \infty} \frac{1}{n} \|\mathbf{x} - \mathbf{g}_{\text{in}}^*(\mathbf{x}(t))\|^2 = \mathbb{E}\{[X - \mathbf{g}_{\text{in}}^*(X + W(t))]^2\}, \quad W(t) \sim \mathcal{N}(0, \tau(t))$$

Run to “convergence” \Rightarrow MSE determined by $\lim_{t \rightarrow \infty} \tau(t)$

Fixed points of Bayes GAMP

$$\lim_{n \rightarrow \infty} \frac{1}{n} \|\mathbf{x} - \mathbf{g}_{\text{in}}^*(\mathbf{x}(t))\|^2 = \mathbb{E}\{[X - \mathbf{g}_{\text{in}}^*(X + W(t))]^2\}, \quad W(t) \sim \mathcal{N}(0, \tau(t))$$

Run to “convergence” \Rightarrow MSE determined by $\lim_{t \rightarrow \infty} \tau(t)$

State evolution

Given $\tau(t)$, compute:

$$\tau^z(t) = \frac{1}{\delta} \text{mmse}(\tau(t))$$

$$\tau(t+1) = \tau^z(t) \left[1 - \frac{1}{\tau(t)} \mathbb{E}\{\text{Var}(Z \mid Z(t), Y)\} \right]^{-1}$$

Fixed points of Bayes GAMP

$$\lim_{n \rightarrow \infty} \frac{1}{n} \|\mathbf{x} - \mathbf{g}_{\text{in}}^*(\mathbf{x}(t))\|^2 = \mathbb{E}\{[X - \mathbf{g}_{\text{in}}^*(X + W(t))]^2\}, \quad W(t) \sim \mathcal{N}(0, \tau(t))$$

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Can determine $\lim_{t \rightarrow \infty} \tau(t)$ via potential function $U(x; \delta)$

Fixed points of Bayes GAMP

$$\tau^z(t) = \frac{1}{\delta} \text{mmse}(\tau(t))$$

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Proposition

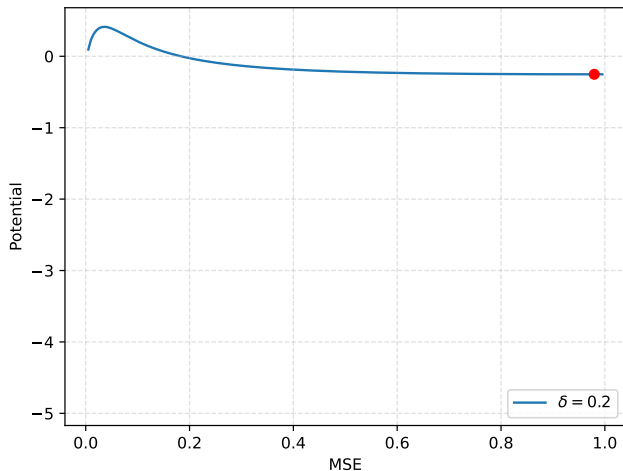
$$\begin{aligned} & \lim_{t \rightarrow \infty} \lim_{n \rightarrow \infty} \frac{1}{n} \|\mathbf{x} - \bar{\mathbf{g}}_{\text{in}}^*(\mathbf{x}(t); t)\|^2 \\ &= \max \left\{ x \in [0, \text{Var}(X)] : \frac{\partial U(x; \delta)}{\partial x} = 0 \right\}. \end{aligned}$$

MSE of Bayes GAMP given by **largest** stationary point of $U(x; \delta)$

Example: Phase Retrieval

$$\mathbf{y} = |\mathbf{Ax}|^2 \quad \text{Prior } P_X(-a) = 0.4, P_X(a) = 0.6$$

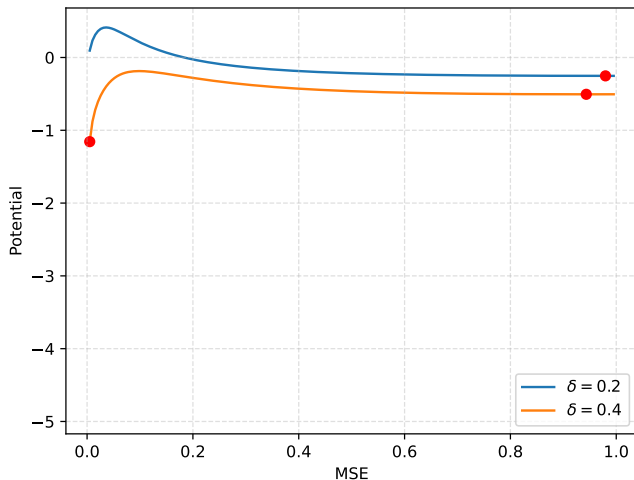
$U(x; \delta)$ vs x



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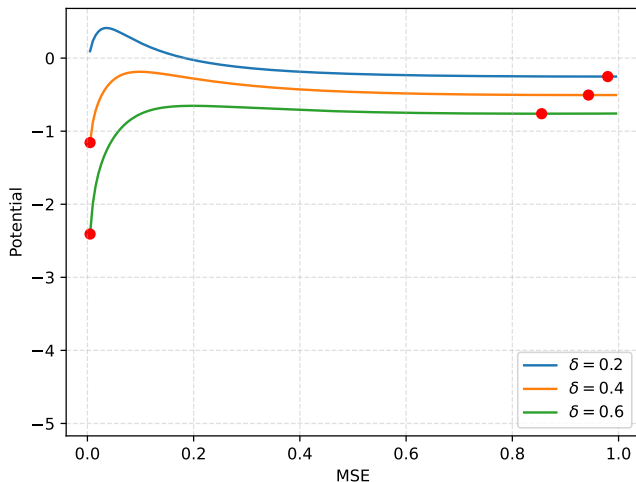
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Example: Phase Retrieval

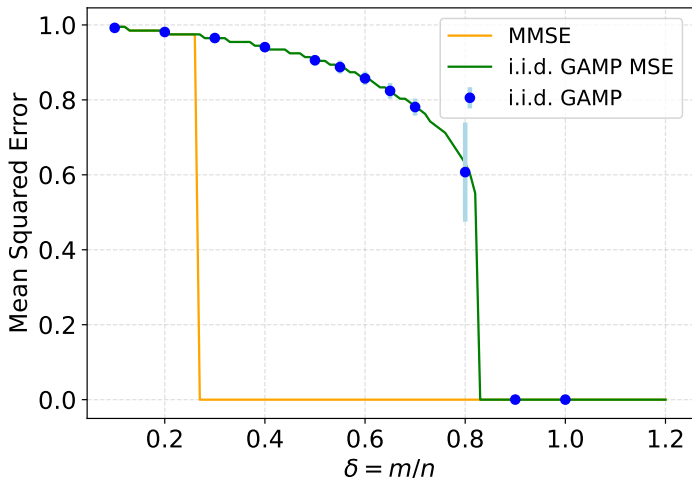
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$U(x; \delta)$ vs x



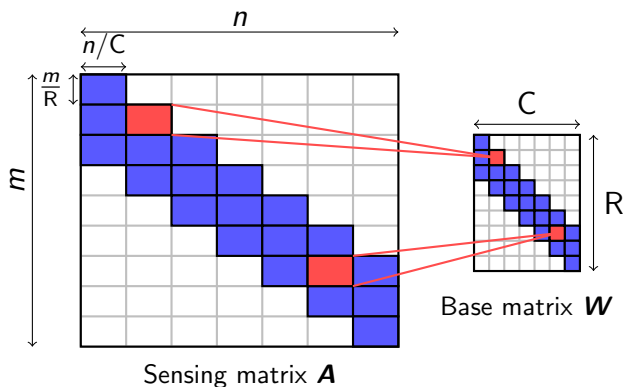
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Can we get the MSE of GAMP to approach global minimum?

Spatially coupled sensing matrix

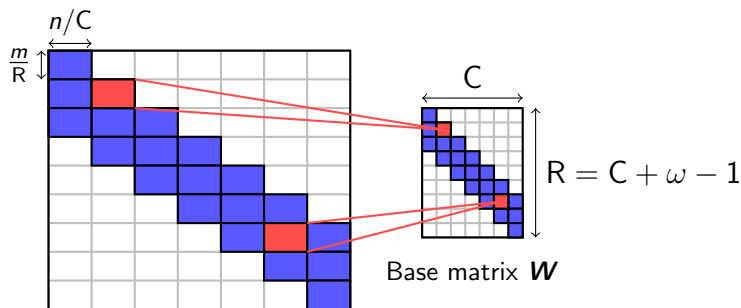
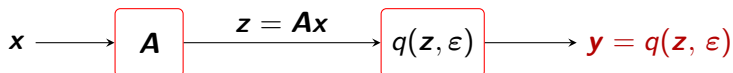


$A_{jk} \sim N(0, W_{rc})$ for $j \in \text{block } r$ and $k \in \text{block } c$

W_{rc} chosen so that each column of \mathbf{A} has $\mathbb{E}[\text{squared-norm}] = 1$

[Donoho, Javanmard, Montanari '13] [Barbier and Krzakala '17] [Liang, Ma and Ping '17] [Hsieh, Rush, V '21] ...

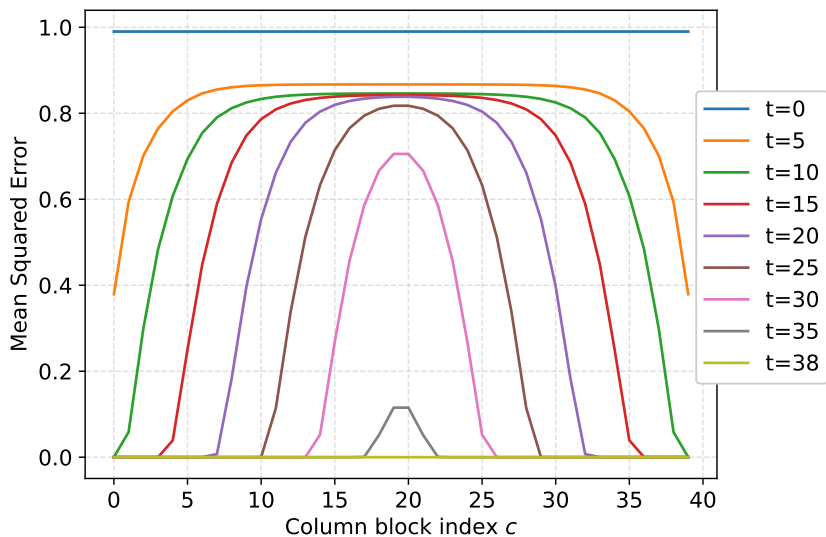
High-level idea



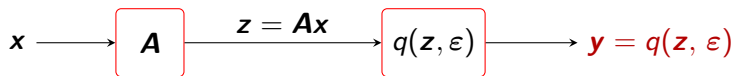
Each little block an iid sensing matrix that multiplies a section of x
First and last sections have observations with less interference \Rightarrow
Can be recovered more easily \Rightarrow helps recover adjacent sections

Decoding wave

Spatially coupled matrix with $C = 40$, $\omega = 6$



Spatially coupled GAMP

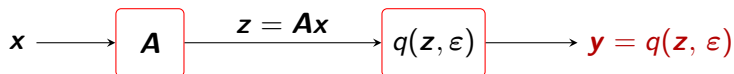


$$\mathbf{x}(t+1) = g_{\text{in}}(\mathbf{x}(t), \mathbf{c}; t) + \boldsymbol{\alpha}^x(t+1) \odot \mathbf{A}^T g_{\text{out}}(\mathbf{z}(t), \mathbf{y}, \mathbf{r}; t)$$

$$\mathbf{z}(t+1) = \mathbf{A} g_{\text{in}}(\mathbf{x}(t+1), \mathbf{c}; t+1) - \boldsymbol{\alpha}^z(t+1) \odot g_{\text{out}}(\mathbf{z}(t), \mathbf{y}, \mathbf{r}; t)$$

- ▶ g_{in} and g_{out} now depend on the column and row section

Spatially coupled GAMP

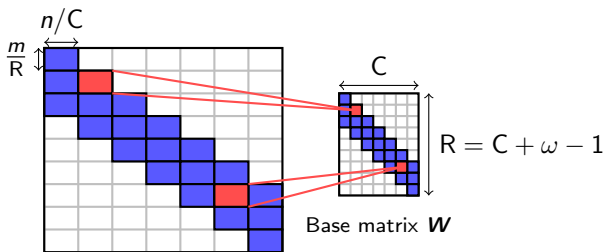


$$\mathbf{x}(t+1) = g_{\text{in}}(\mathbf{x}(t), \mathbf{c}; t) + \boldsymbol{\alpha}^{\mathbf{x}}(t+1) \odot \mathbf{A}^{\text{T}} g_{\text{out}}(\mathbf{z}(t), \mathbf{y}, \mathbf{r}; t)$$

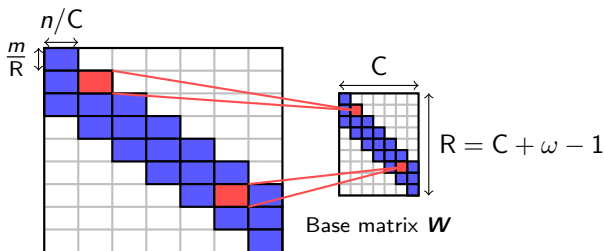
$$\mathbf{z}(t+1) = \mathbf{A} g_{\text{in}}(\mathbf{x}(t+1), \mathbf{c}; t+1) - \boldsymbol{\alpha}^{\mathbf{z}}(t+1) \odot g_{\text{out}}(\mathbf{z}(t), \mathbf{y}, \mathbf{r}; t)$$

- ▶ g_{in} and g_{out} now depend on the column and row section
- ▶ $\boldsymbol{\alpha}^{\mathbf{x}}(t+1) = [\alpha_1^{\mathbf{x}}(t+1), \dots, \alpha_{\mathbf{C}}^{\mathbf{x}}(t+1)]$
- ▶ $\boldsymbol{\alpha}^{\mathbf{z}}(t+1) = [\alpha_1^{\mathbf{z}}(t+1), \dots, \alpha_{\mathbf{R}}^{\mathbf{z}}(t+1)]$

Asymptotics of SC-GAMP



Asymptotics of SC-GAMP



The empirical distribution of $(\mathbf{x}_c, \mathbf{x}_c(t))$ converges to the law of

$$[X, X + W_c(t)], \quad \text{where } W(t) \sim N(0, \tau_c(t))$$

for $c = 1, \dots, C$

The empirical distribution of $(\mathbf{z}_r, \mathbf{z}_r(t))$ converges to the law of

$$[Z_r, Z_r(t)] \sim N(0, \Lambda_r(t))$$

for $r = 1, \dots, R$

SC-GAMP Performance

State evolution has $C + R$ parameters:

$$\{\tau_1(t), \dots, \tau_C(t), \Lambda_1(t), \dots, \Lambda_R(t)\} \longrightarrow \\ \{\tau_1(t+1), \dots, \tau_C(t+1), \Lambda_1(t+1), \dots, \Lambda_R(t+1)\}$$

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Theorem (Asymptotic MSE): For $t \geq 1$

$$\lim_{n \rightarrow \infty} \frac{1}{n} \|\mathbf{x} - \mathbf{g}_{\text{in}}^*(\mathbf{x}(t))\|^2 = \frac{1}{C} \sum_{c=1}^C \mathbb{E}\{ [X - \mathbf{g}_{\text{in}}^*(X + W_c(t), c)]^2 \}$$

where $W_c(t) \sim N(0, \tau_c(t))$

Fixed points of Bayes SC-GAMP

$$\lim_{n \rightarrow \infty} \frac{1}{n} \|\mathbf{x} - \mathbf{g}_{\text{in}}^*(\mathbf{x}(t))\|^2 = \frac{1}{C} \sum_{c=1}^C \mathbb{E}\{ [X - g_{\text{in}}^*(X + W_c(t), c)]^2 \}$$

where $W_c(t) \sim N(0, \tau_c(t))$

Run SC-GAMP to convergence \Rightarrow MSE determined by

$$\lim_{t \rightarrow \infty} \{\tau_1(t), \dots, \tau_C(t)\}$$

How to determine fixed points of this **coupled** recursion?

Fixed points of Bayes SC-GAMP

$$\lim_{n \rightarrow \infty} \frac{1}{n} \|\mathbf{x} - \mathbf{g}_{\text{in}}^*(\mathbf{x}(t))\|^2 = \frac{1}{C} \sum_{c=1}^C \mathbb{E}\{ [X - \mathbf{g}_{\text{in}}^*(X + W_c(t), c)]^2 \}$$

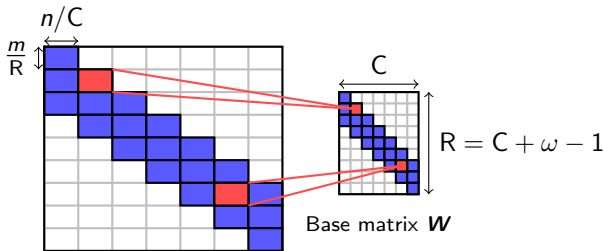
where $W_c(t) \sim \mathcal{N}(0, \tau_c(t))$

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How to determine fixed points of this **coupled** recursion?

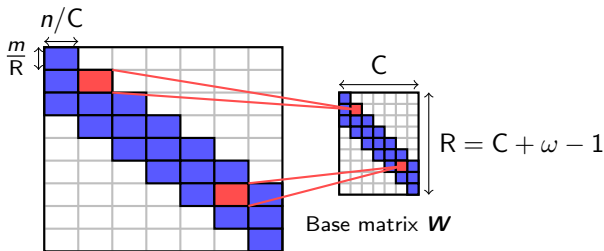
[Yedla, Jian, Nguyen, Pfister '14]: *A simple proof of Maxwell saturation for coupled scalar recursions*



Theorem (Fixed point of SC-GAMP): Fix $\gamma > 0$. Then for $\omega > \omega_0$ and $t > t_0$:

$$\begin{aligned} & \lim_{n \rightarrow \infty} \frac{1}{n} \|\mathbf{x} - \mathbf{g}_{\text{in}}^*(\mathbf{x}(t); t)\|^2 \\ & \leq \left(\arg \min_{x \in [0, \text{Var}(X)]} U(x; \delta_{\text{in}}) + \gamma \right) \frac{C + \omega}{C}. \end{aligned}$$

Here $\delta_{\text{in}} = \delta_{\frac{C}{R}}$ is the inner sampling ratio.



Corollary (Bayes optimality of SC-GAMP): Fix $\epsilon > 0$. Then for $\omega > \omega_0$, sufficiently large C and $t > t_0$ we have:

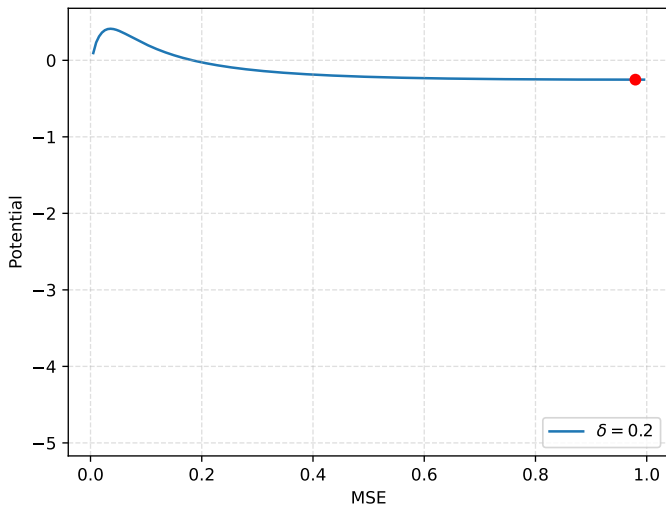
$$\lim_{n \rightarrow \infty} \frac{1}{n} \|\mathbf{x} - \mathbf{g}_{\text{in}}^*(\mathbf{x}(t); t)\|^2 \leq \arg \min_{\mathbf{x} \in [0, \text{Var}(X)]} U(\mathbf{x}; \delta) + \epsilon.$$

Analogous to threshold saturation in SC-LDPC codes

Example: Phase Retrieval

$$\mathbf{y} = |\mathbf{Ax}|^2 \quad \text{Prior } P_X(-a) = 0.4, P_X(a) = 0.6$$

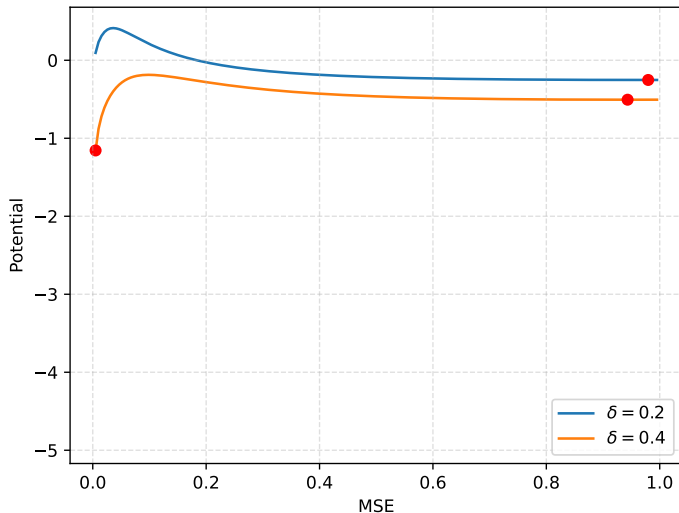
$U(x; \delta)$ vs x



Example: Phase Retrieval

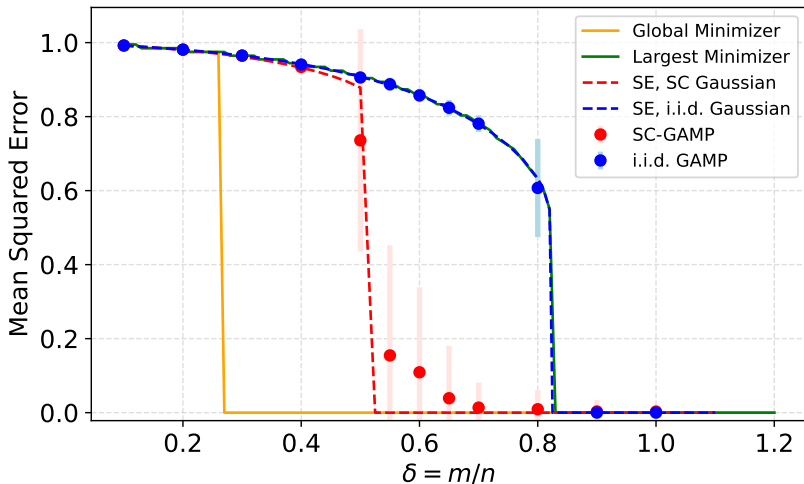
$$\mathbf{y} = |\mathbf{Ax}|^2 \quad \text{Prior } P_X(-a) = 0.4, P_X(a) = 0.6$$

$U(x; \delta)$ vs x



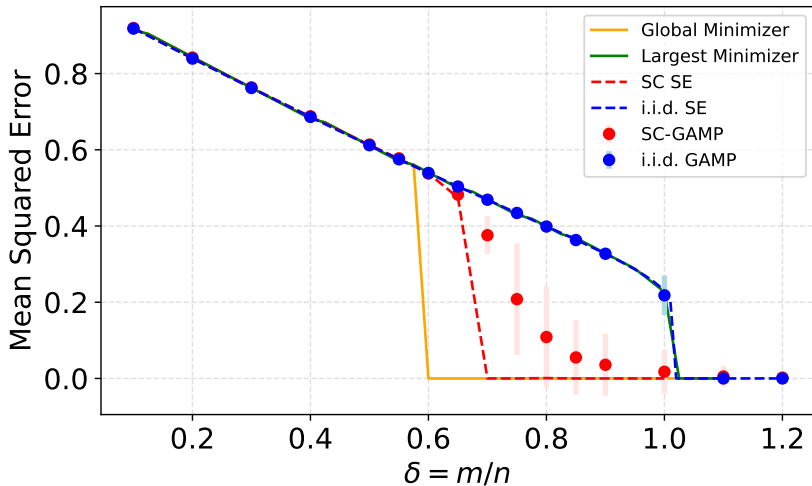
Phase retrieval

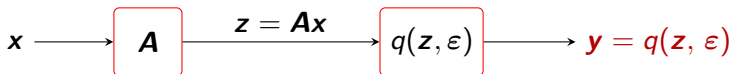
$$\mathbf{y} = |\mathbf{Ax}|^2 \quad \text{Prior } P_X(-a) = 0.4, P_X(a) = 0.6$$



ReLU model

$$y = \max(\mathbf{Ax}, 0) \quad \text{Prior } P_X(-b) = P_X(b) = 0.25, P_X(0) = 0.5$$





Performance of optimal estimator with iid Gaussian design achieved by *spatially coupled design with message passing estimator*

Future directions

Spatial coupling with *structured* random matrices

- E.g., Fourier, DCT, Hadamard based matrices
- Enables faster AMP-like algorithms

Spatial coupling for variants of group testing