Understanding Phase Transitions via Mutual Information and MMSE

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Bayes Optimal Inference

Distribution $p(\boldsymbol{x}, \boldsymbol{y})$ on random vectors (matrices, tensors)

$$\begin{aligned} \text{unknown:} \qquad & \boldsymbol{X} = (X_1, \dots, X_n) \\ \text{observed data:} \qquad & \boldsymbol{Y} = (Y_1, \dots, Y_m) \end{aligned}$$

Posterior distribution of unknowns:

$$p(\boldsymbol{x} \,|\, \boldsymbol{y}) = \frac{p(\boldsymbol{y} \,|\, \boldsymbol{x}) p(\boldsymbol{x})}{p(\boldsymbol{y})}.$$

Basic questions:

1. What are the fundamental limits of inference?
2. Can we achieve these limits using efficient methods?

Marginals and Moments of Posterior Distribution

- Marginal of (random) posterior on set of indices $S \subset [n]$,

$$p(\boldsymbol{x}_S \mid \boldsymbol{Y}) = \int p(\boldsymbol{x} \mid \boldsymbol{Y}) \, \mathrm{d}\boldsymbol{x}_{S^c}$$

- Mean and covariance of (random) posterior distribution

$$\mathbb{E}[\boldsymbol{X} \mid \boldsymbol{Y}] = \int \boldsymbol{x} \, p(\boldsymbol{x} \mid \boldsymbol{Y}) \, \mathrm{d}\boldsymbol{x}$$

$$\mathsf{Cov}(\boldsymbol{X} \mid \boldsymbol{Y}) = \mathbb{E}\big[(\boldsymbol{X} - \mathbb{E}[\boldsymbol{X} \mid \boldsymbol{Y}])(\boldsymbol{X} - \mathbb{E}[\boldsymbol{X} \mid \boldsymbol{Y}])^T \mid \boldsymbol{Y}\big]$$

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- Minimum mean-squared error (MMSE)

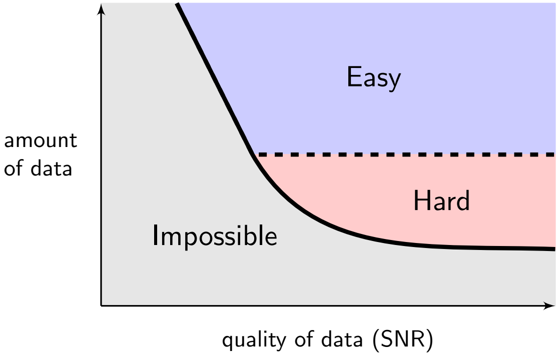
$$\mathsf{mmse}(\boldsymbol{X} \mid \boldsymbol{Y}) = \mathbb{E}\Big[\|\boldsymbol{X} - \mathbb{E}[\boldsymbol{X} \mid \boldsymbol{Y}]\|^2\Big] = \mathbb{E}[\mathrm{tr}(\mathsf{Cov}(\boldsymbol{X} \mid \boldsymbol{Y}))]$$

  Also known as Bayes risk under squared-error loss

Approaches to Analysis

- **Information Theory**
  - Single-letter formulas describe fundamental limits
  - Models with structured randomness: e.g., Markov sources (compression) and finite-state channels (communication)
- **Replica Method from Statistical Physics**
  - Conjectured single-letter formulas via heuristics
  - Models with disordered randomness: e.g., spin glasses and modern high-dimensional inference problems
- **Approximate Inference**
  - Fixed-points of message passing algorithms related stationary points of potential functions.

Phase Diagram for High-Dimensional Inference



Easy – Computationally efficient methods succeed.

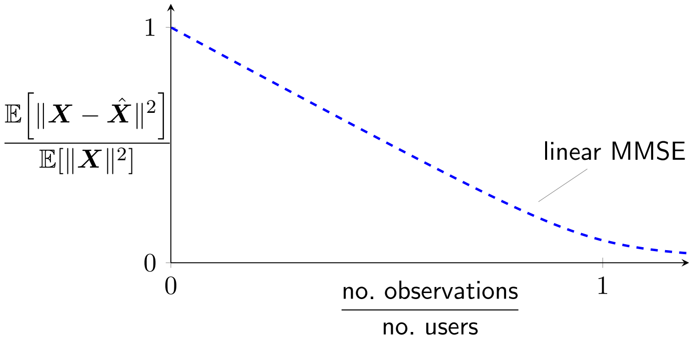
Hard – All known efficient methods fail but intractable methods succeed.

Impossible – All methods fail, regardless of complexity.

Example: Multiuser Detection in CDMA

$$\boldsymbol{Y} = \sum_j \boldsymbol{A}_j X_j + \boldsymbol{W}, \qquad \boldsymbol{W} \sim \mathcal{N}(0, \sigma^2 I)$$

- $\{\boldsymbol{A}_j\}$ are known signature vectors with IID entries
- $\{X_j\}$ are IID $\{+1, -1\}$ messages



Tse,Hanly'99, Verdu,Shamai'99,

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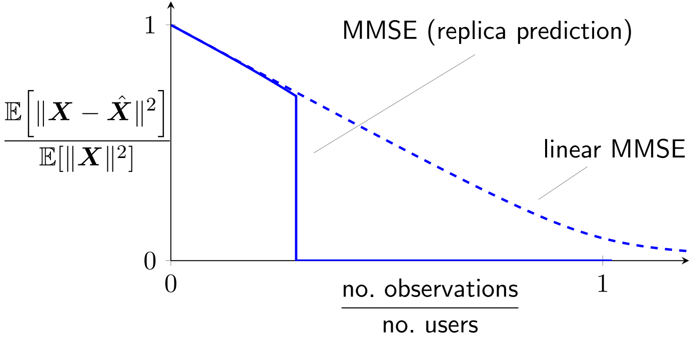

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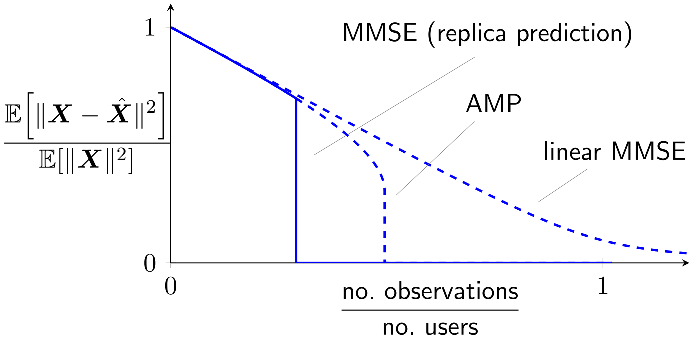
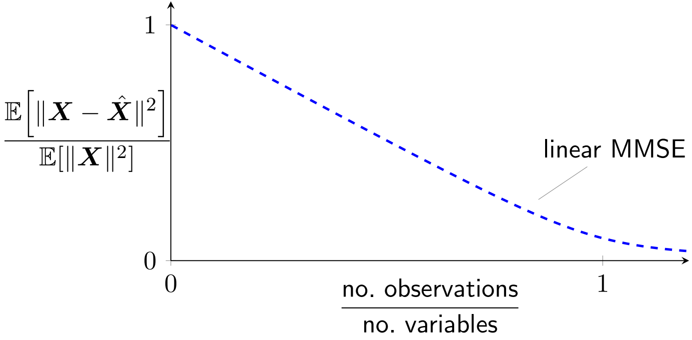


Tse,Hanly'99, Verdu,Shamai'99, Tanaka'02, Guo,Verdu'05, Bayati,Montanari'11

Example: Compressed Sensing

$$\boldsymbol{Y} = \sum_j \boldsymbol{A}_j X_j + \boldsymbol{W}, \qquad \boldsymbol{W} \sim \mathcal{N}(0, \sigma^2 I)$$

- $\{\boldsymbol{A}_j\}$ are columns of known sensing matrix with IID entries
- $\{X_j\}$ are IID Bernoulli-Gaussian: $p(x) = (1-\epsilon)\delta_0(x) + \epsilon\mathcal{N}(x \mid 0, \epsilon^{-1})$



Donoho,Maleki,Montanari'09, Bayati,Montanari'11, R,Gastpar'12

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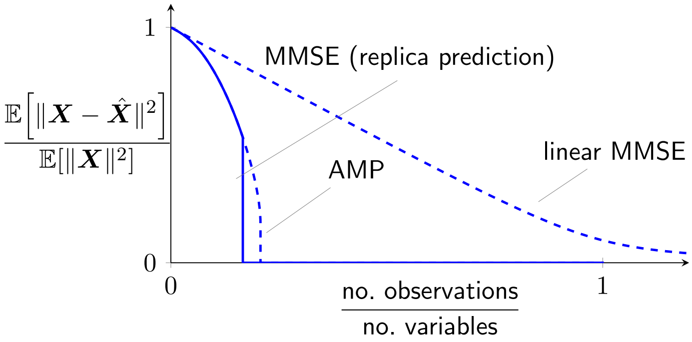

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Motivating Questions

- Where do these formulas come from?
- When is AMP optimal?
- Are the replica predictions correct?
- What about other models?

Signal-Plus Noise Model (Scalar Case)

$$Y = \sqrt{s}X + Z, \qquad X \sim p(x), \qquad Z \sim \mathcal{N}(0,1)$$

Guo,Shamai,Verdu'05, R,Pfister,Dytso'18

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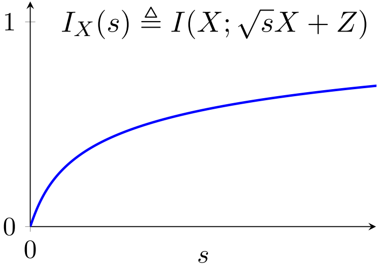

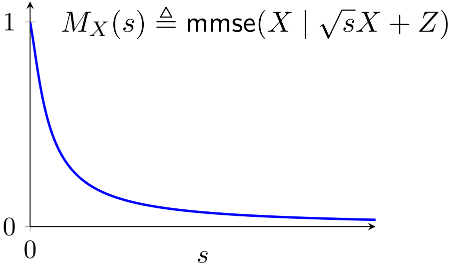

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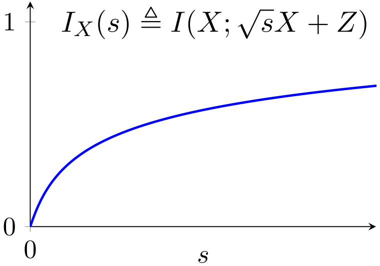
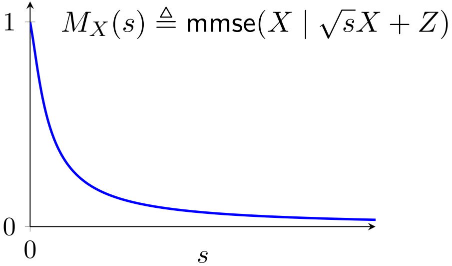
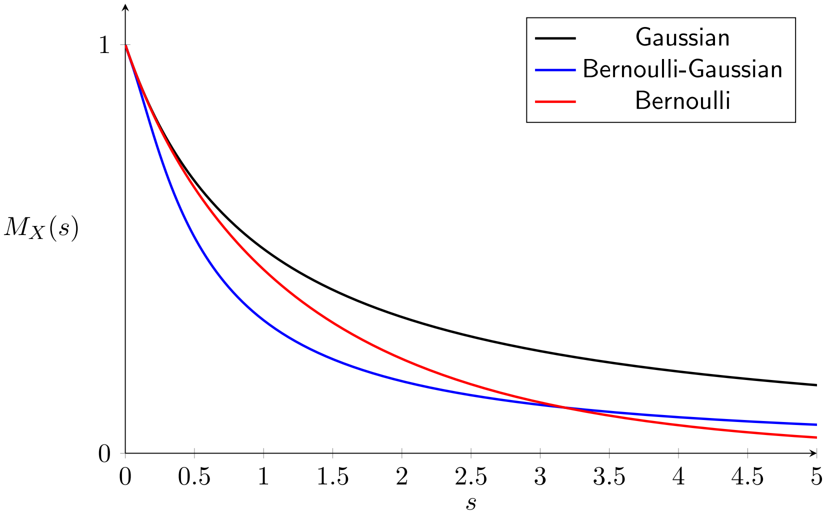




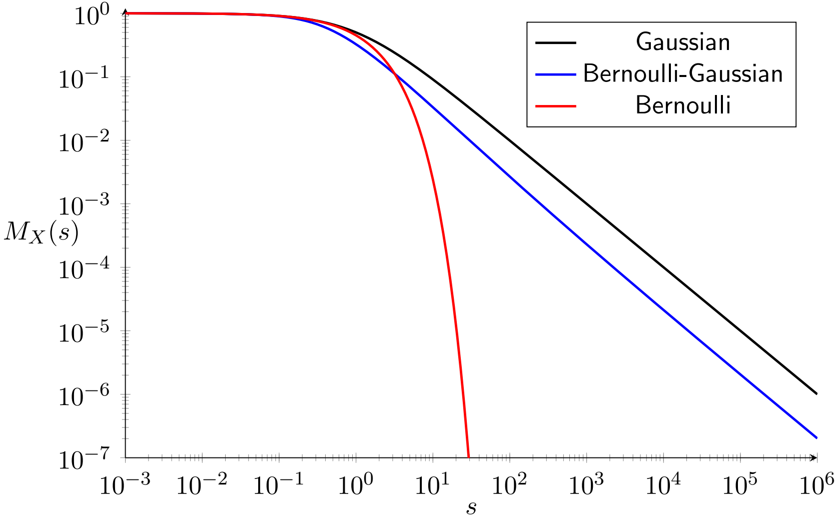
I-MMSE Relation: $\frac{\mathrm{d}}{\mathrm{d}s} I_X(s) = \frac{1}{2} M_X(s)$

Guo,Shamai,Verdu'05, R,Pfister,Dytso'18

Effect of Signal Prior on MMSE Function



Effect of Signal Prior on MMSE Function (Log Scale)



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Experiment: Linear Regression with IID Gaussian matrix

- Length $n = 10^4$ vector $\boldsymbol{X}$ with IID Bernoulli-Gaussian entries

$$X_i \sim p(x) = 0.8\,\delta_0(x) + 0.2\,\mathcal{N}(x \mid 0, 5)$$

- Observations $\boldsymbol{Y} \in \mathbb{R}^m, \boldsymbol{A} \in \mathbb{R}^{m \times n}$ with SNR $=$ 60 dB

$$\boldsymbol{Y} \sim \mathcal{N}(\boldsymbol{A}\boldsymbol{X}, 10^{-6} I_m), \qquad A_{ij} \sim \mathcal{N}(0, 1/n)$$

Donoho,Maleki,Montanari'09, Matlab implementation by Schniter et. al.

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$$\boldsymbol{Y} \sim \mathcal{N}(\boldsymbol{A}\boldsymbol{X}, 10^{-6} I_m), \qquad A_{ij} \sim \mathcal{N}(0, 1/n)$$

- Use AMP to approximate marginals of posterior: $\hat{p}(x_i \mid \boldsymbol{Y}, \boldsymbol{A})$

AMP squared error: $$\frac{1}{n}\sum_{i=1}^{n}(X_i - \mathbb{E}_{\hat{p}}[X_i \mid \boldsymbol{Y}, \boldsymbol{A}])^2$$

AMP posterior variance: $$\frac{1}{n}\sum_{i=1}^{n}\mathsf{Var}_{\hat{p}}(X_i i \mid \boldsymbol{Y}, \boldsymbol{A}).$$

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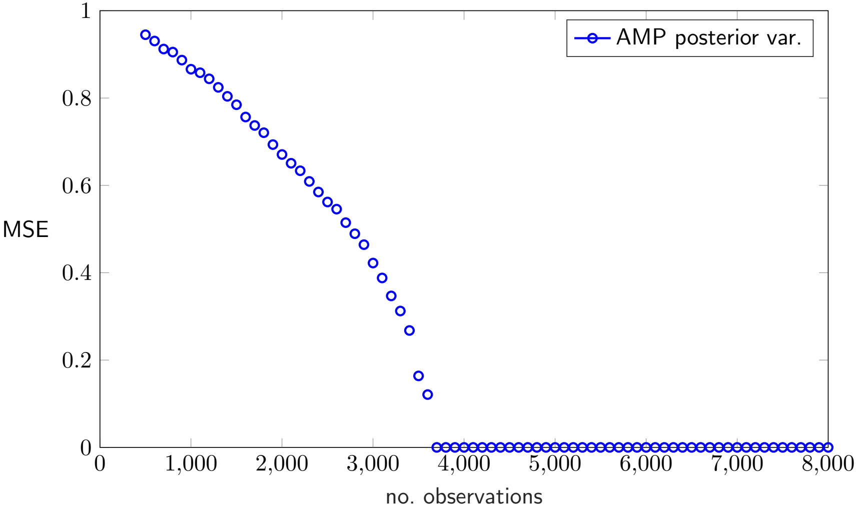

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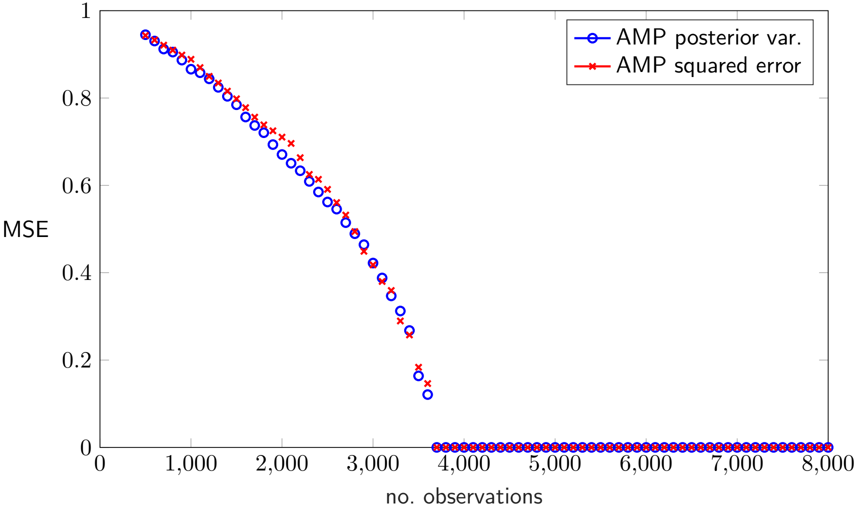

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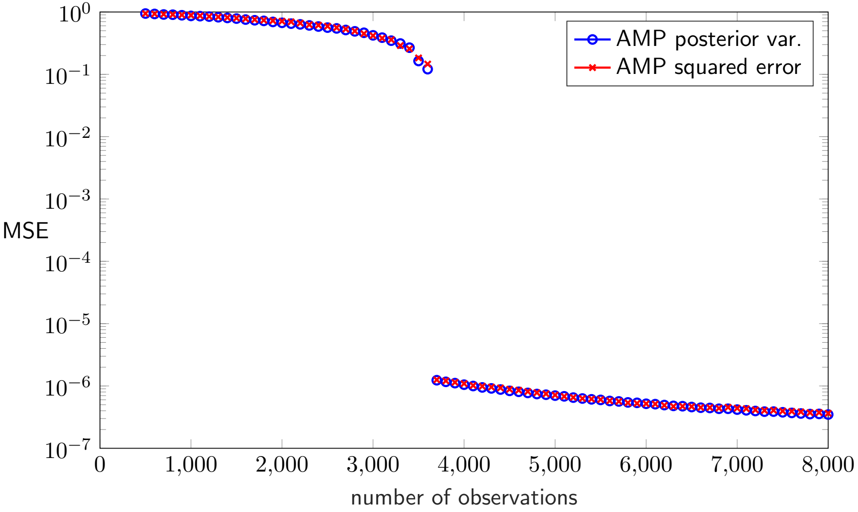
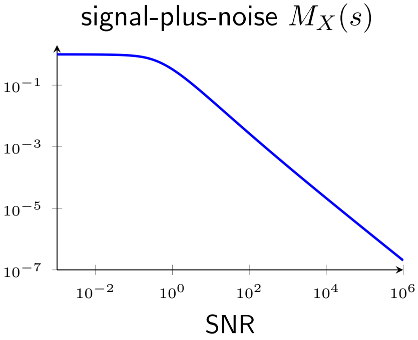


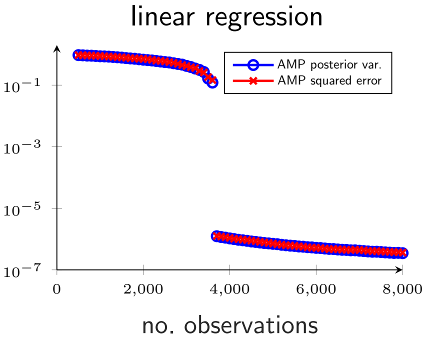
Motivating Questions

- Why is there a big change in behavior around 3,500 observations?
- Do AMP estimates correspond to true posterior distribution?

MSE of AMP

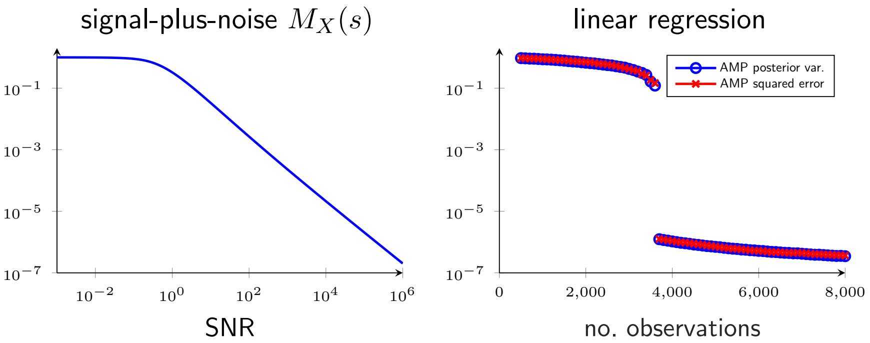


signal-plus-noise $M_X(s)$
10^{-1}
10^{-3}
10^{-5}
10^{-7}
10^{-2}
10^{0}
10^{2}
10^{4}
10^{6}
SNR



linear regression
AMP posterior var.
AMP squared error
10^{-1}
10^{-3}
10^{-5}
10^{-7}
0
2,000
4,000
6,000
8,000
no. observations

MSE of AMP



Define asymptotic MSE

$$\mathcal{E}_{\mathsf{AMP}}(\delta) \triangleq \lim_{m,n\to\infty} \frac{1}{n}\mathbb{E}\left[\left\|\boldsymbol{X} - \hat{\boldsymbol{X}}_{\mathsf{AMP}}\right\|^2\right], \qquad m/n \to \delta$$

State Evolution for AMP

Recall rom Phil's talk, the AMP per-iteration MSE $\mathcal{E}^t$ satisfies

$$\mathcal{E}^{t+1} = M_X\left(\frac{\delta}{\sigma^2 + \mathcal{E}^t}\right), \qquad \delta = m/n$$

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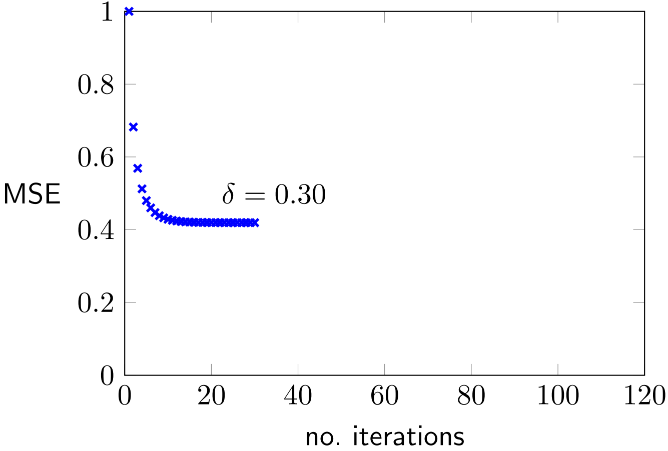

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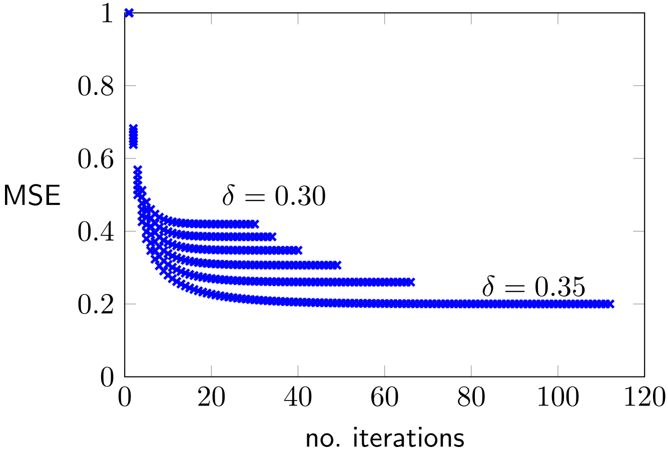

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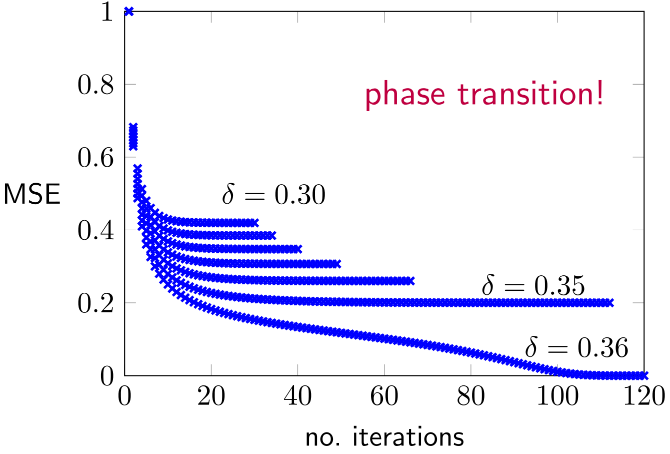

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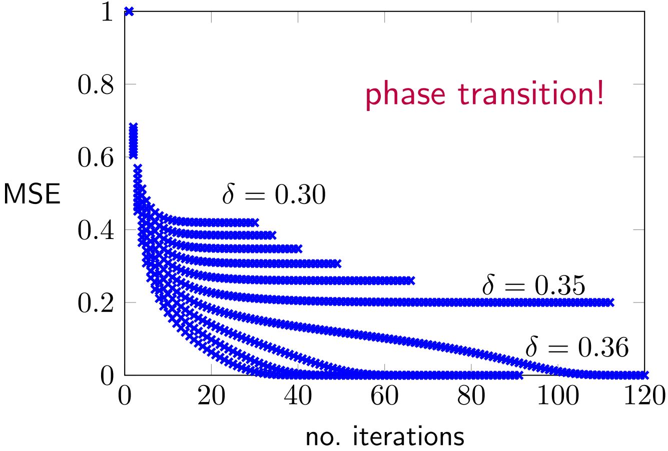
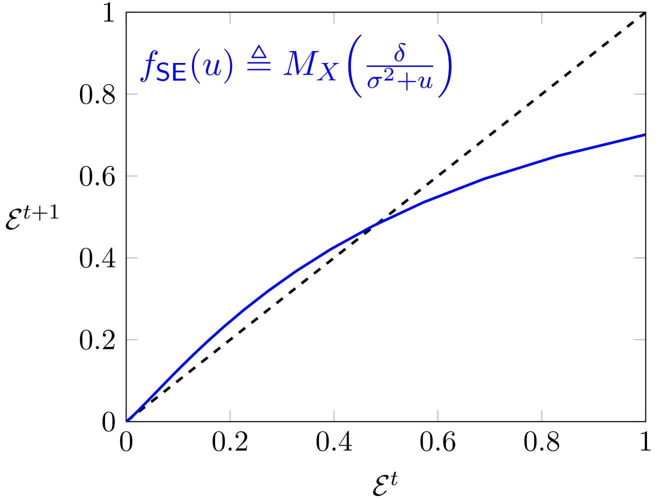


Fixed-Point Analysis of State Evolution



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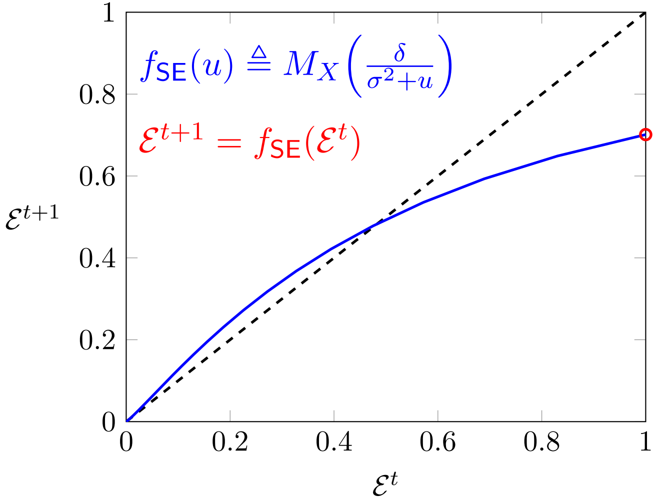

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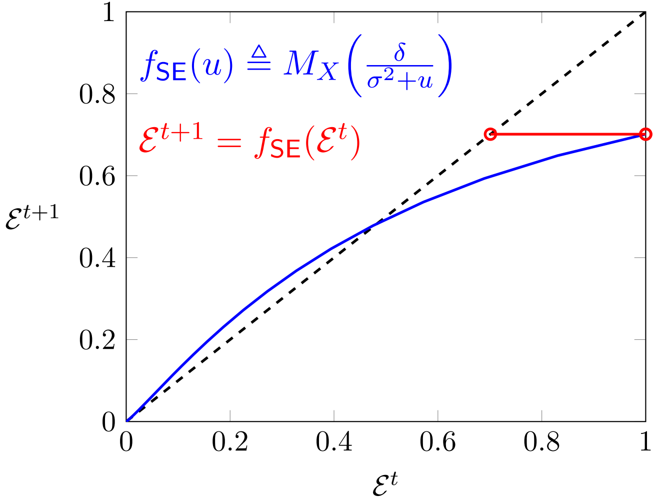

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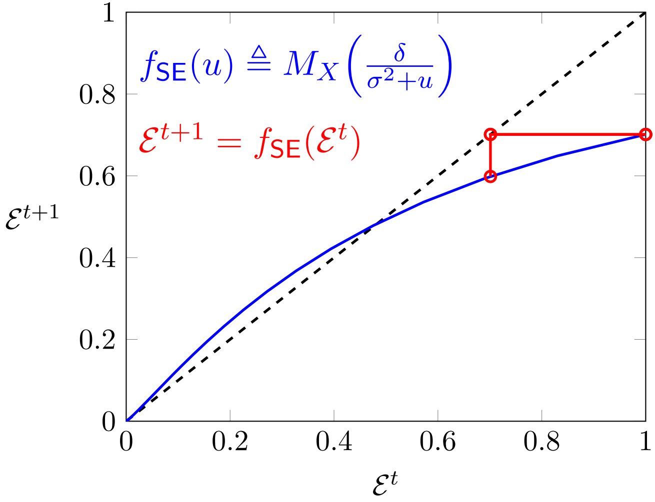

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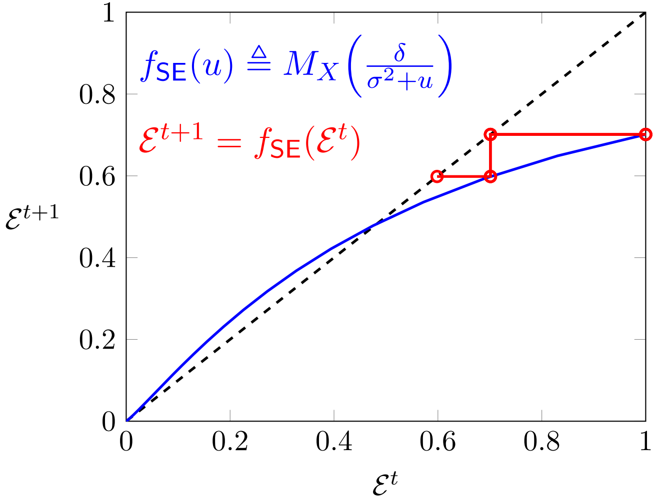

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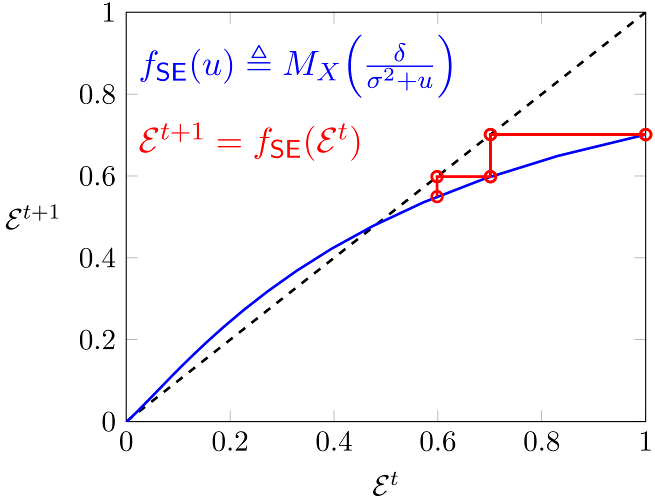

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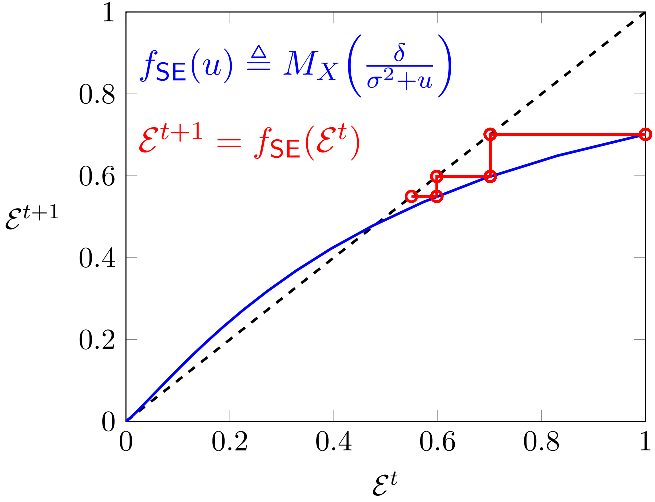

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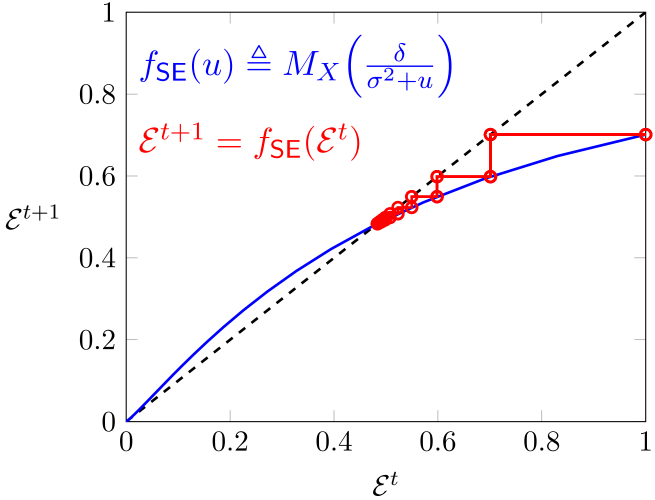

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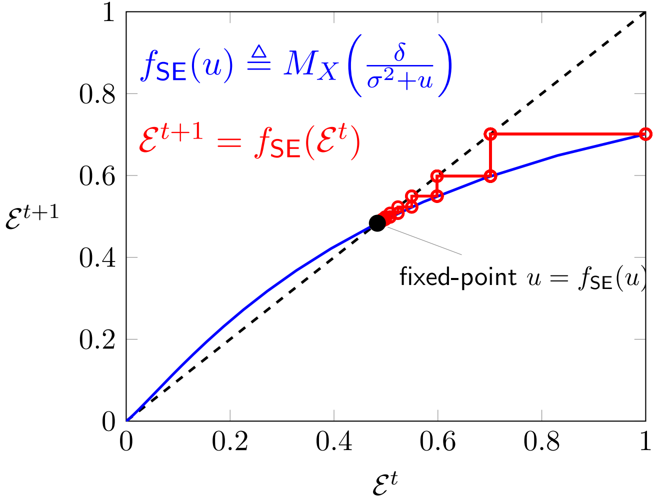

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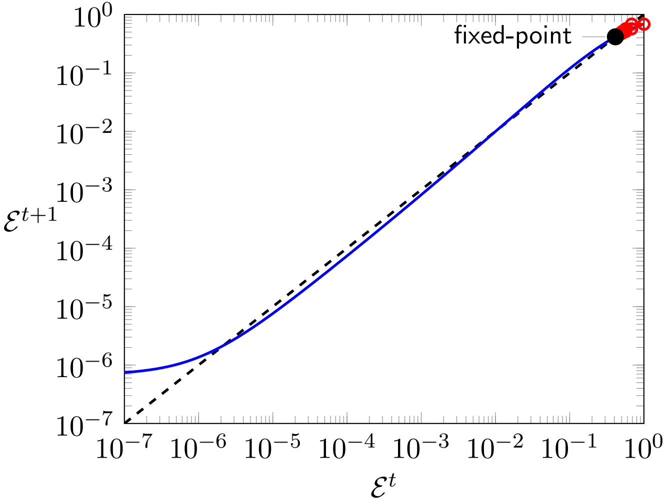

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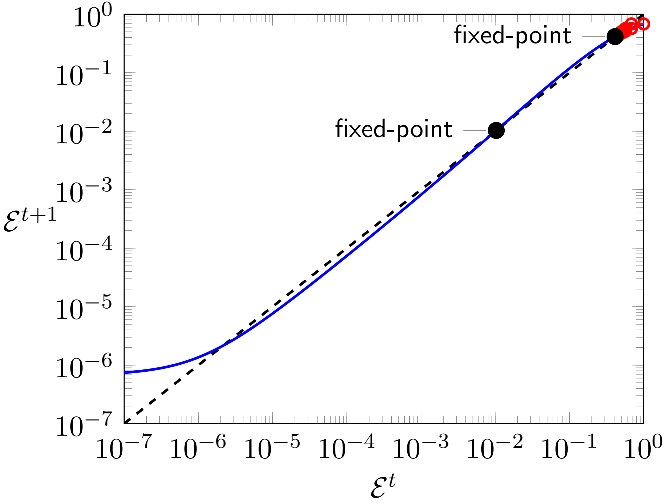

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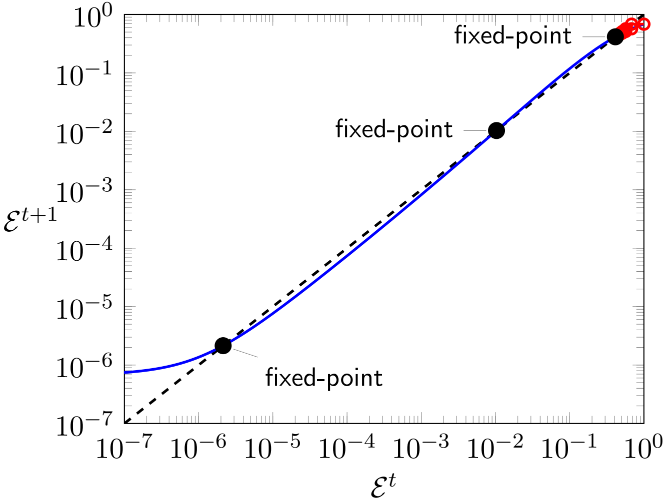

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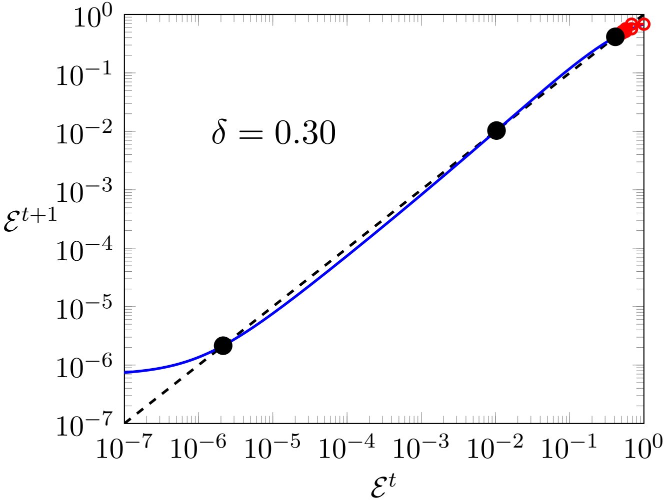

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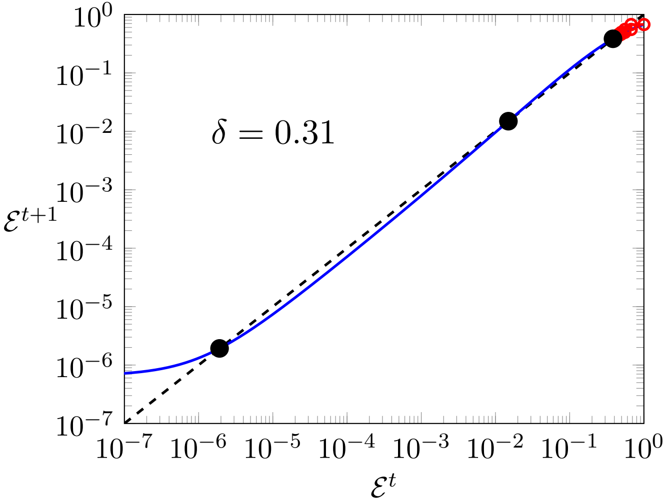

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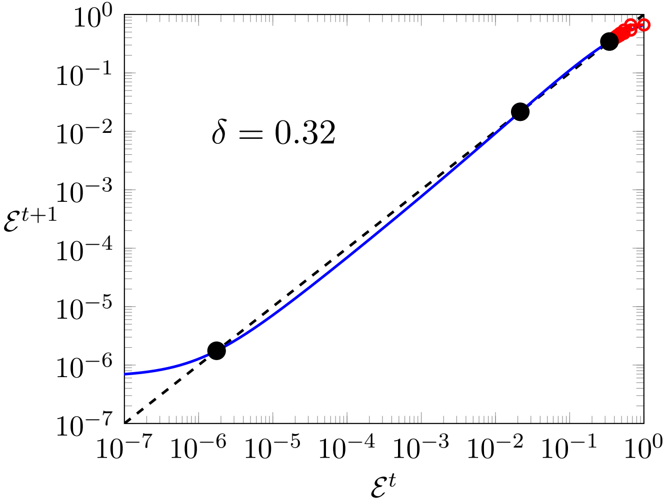

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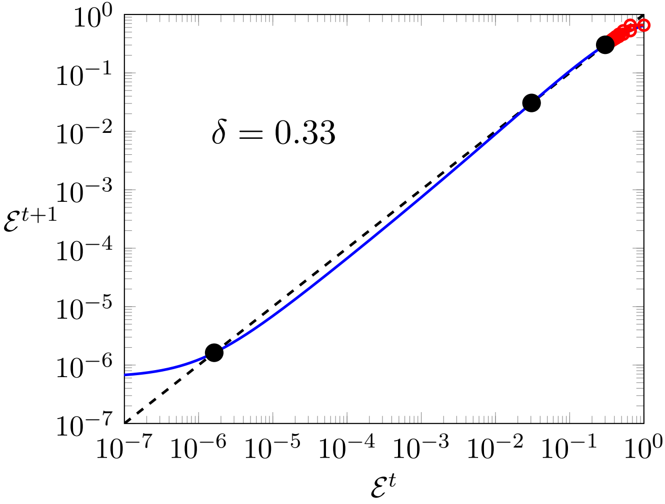

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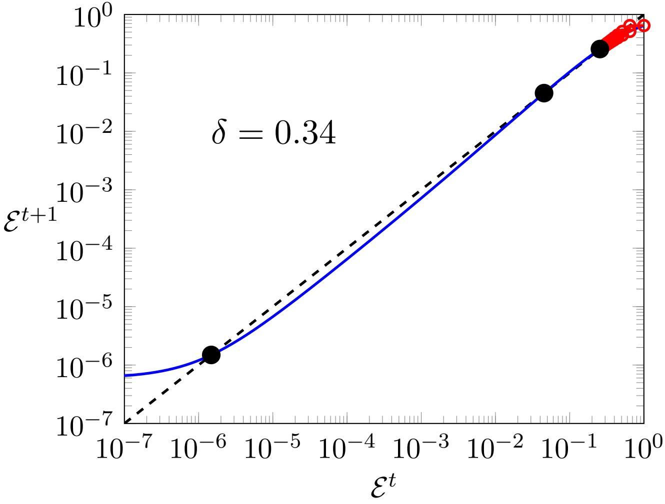

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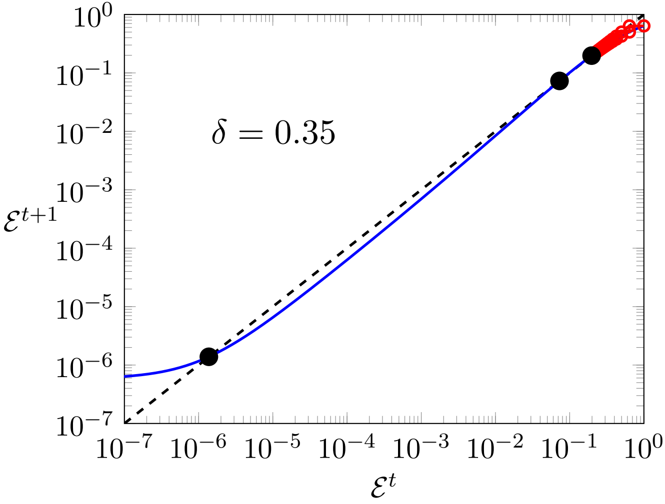

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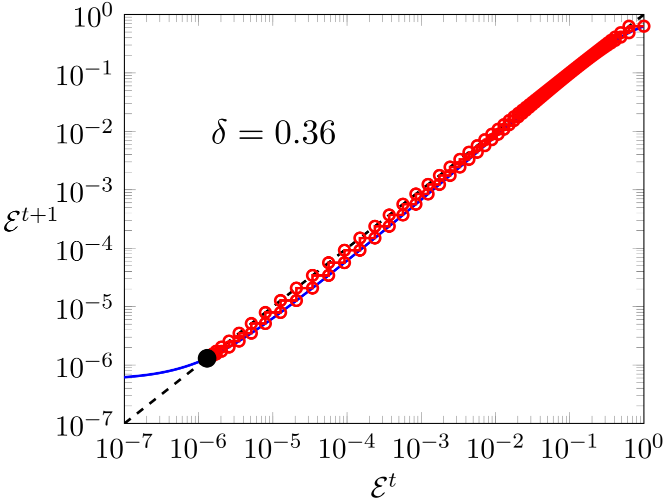
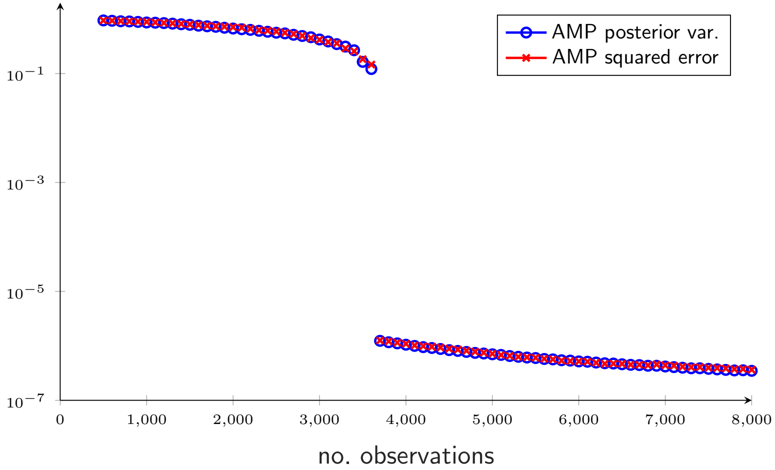


AMP MSE is Upper Envelope of Fixed-Point Curve



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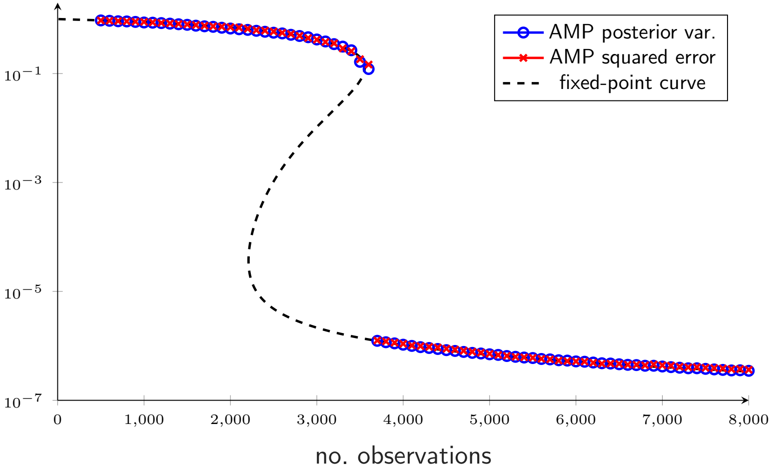

$$\mathcal{E}_{\mathrm{AMP}}(\delta) = \max\left\{ u \,:\, u = M_X\left(\frac{\delta}{\sigma^2 + u}\right)\right\}$$

Asymptotic Mutual Information and MMSE

$$\mathcal{I}(\delta) \triangleq \lim_{\substack{m,n\to\infty \\ m/n\to\delta}} \frac{1}{n} I(\boldsymbol{X};\boldsymbol{Y}\,|\,\boldsymbol{A})$$

$$\mathcal{E}(\delta) \triangleq \lim_{\substack{m,n\to\infty \\ m/n\to\delta}} \frac{1}{n}\,\mathsf{mmse}(\boldsymbol{X}\,|\,\boldsymbol{Y},\boldsymbol{A}).$$

Replica-Symmetric Formulas

Recall scalar mutual information function

$$I_X(s) = \frac{1}{2} \int_0^s M_X(s') \, \mathrm{d}s'$$

Replica-Symmetric Formulas

Recall scalar mutual information function

$$I_X(s) = \frac{1}{2}\int_0^s M_X(s')\,\mathrm{d}s'$$

Consider potential function:

$$\mathcal{F}_\delta(u) \triangleq I_X\left(\frac{\delta}{\sigma^2+u}\right) + \frac{\delta}{2}\left(\log\left(1+\frac{u}{\sigma^2}\right) - \frac{u}{\sigma^2+u}\right)$$

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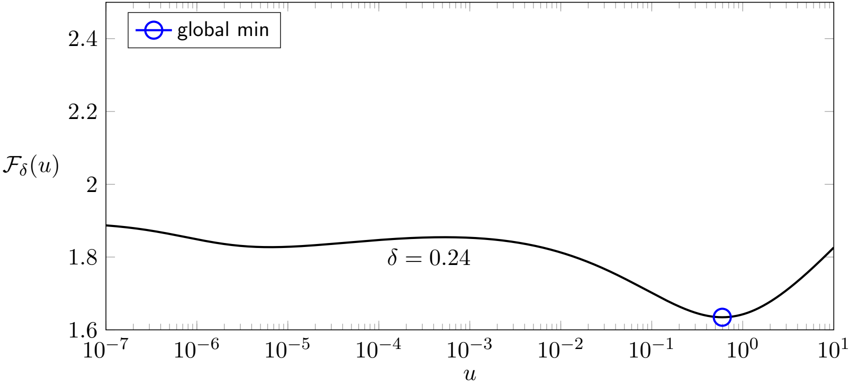
RS formulas defined by global minimum

$$\mathcal{I}_{\mathsf{RS}}(\delta) \triangleq \min_u \mathcal{F}_\delta(u)$$

$$\mathcal{E}_{\mathsf{RS}}(\delta) \triangleq \arg\min_u \mathcal{F}_\delta(u)$$

RS MMSE is Global Minimizer of Potential Function



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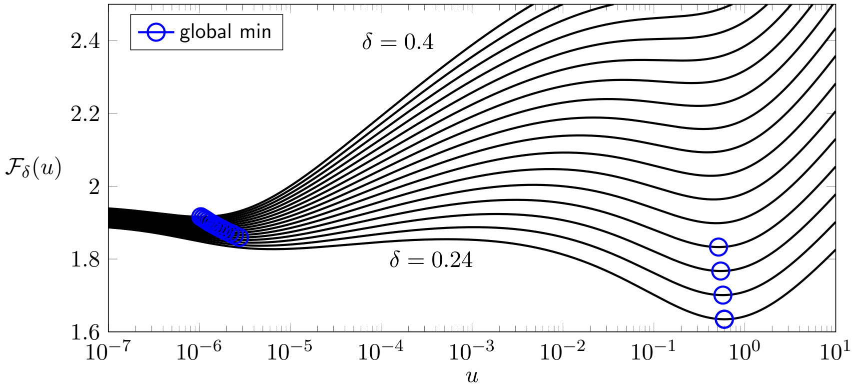

Potential Function view of AMP MSE.

By I-MMSE relation, one finds that the stationary points of potential function satisfy fixed-point equation

$$\mathcal{F}'_\delta(u) = 0 \quad \iff \quad u = M_X\left(\frac{\delta}{\sigma^2 + u}\right)$$

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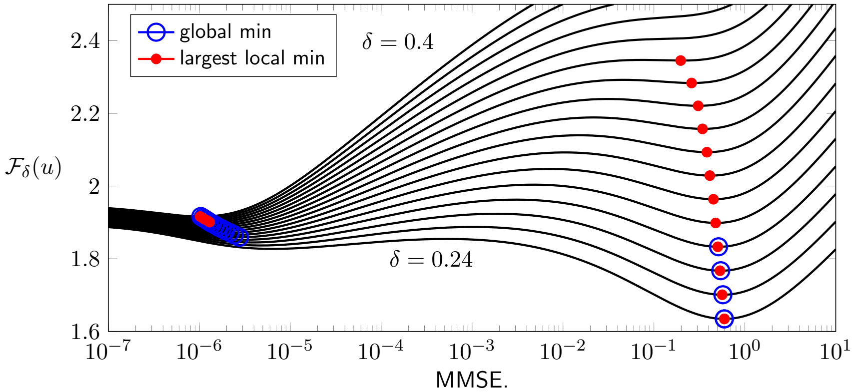
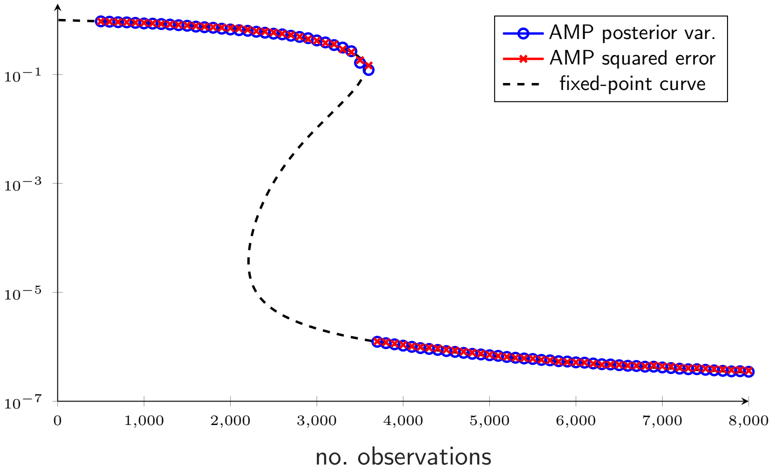
Hence, MSE of AMP is largest local minimizer:

$$\mathcal{E}_{\mathrm{AMP}}(\delta) = \max\left\{u \,:\, \mathcal{F}_\delta'(u) = 0\right\}$$

AMP MSE is Largest Local Minimizer



RS Formula for MMSE



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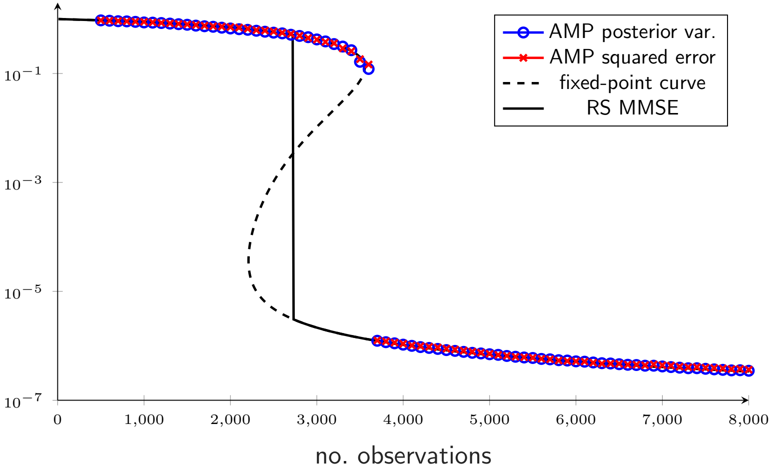

Rigorous Proofs of RS Formula

- Derived using heuristic replica method from statistical physics Tanaka 2001, Guo and Verdu 2005
- First proof by R and Pfister 2016
- Alternate proof using a different method Barbier, Dia, Macris, Krzakala, 2016

Recap of Main Points

- MSE of AMP given by largest solution to fixed-point equation

$$\mathcal{E}_{\mathrm{AMP}}(\delta) = \max\left\{u \,:\, u = M_X\left(\frac{\delta}{\sigma^2 + u}\right)\right\}$$

- MMSE is given by minimum energy solution to fixed-point equation

$$\mathcal{E}(\delta) = \arg\min_u \left\{ I_X\left(\frac{\delta}{\sigma^2 + u}\right) + \frac{\delta}{2}\left(\log\left(1 + \frac{u}{\sigma^2}\right) - \frac{u}{\sigma^2 + u}\right)\right\}$$

- Hence, AMP is optimal if and only if the largest solution is also the minimum energy solution.

- Phase transition: when the solution jump from one location to another.

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Proof I: New Observations are Approx. Gaussian

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- Let $Y^i = (Y_1, \ldots, Y_i)$ and apply chain rule

$$I(\boldsymbol{X}, \boldsymbol{Y} \mid \boldsymbol{A}) = \sum_{i=0}^{m-1} \underbrace{I(\boldsymbol{X}; Y_{i+1} \mid Y^i, \boldsymbol{A})}_{\text{info. from new obs.}}$$

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- If $p(\boldsymbol{x} \mid Y^i, \boldsymbol{A})$ is weakly correlated, then $Y_{i+1} \mid Y^i, \boldsymbol{A}$ is approx. Gaussian:

$$\begin{aligned} Y_{i+1} - \mathbb{E}\big[Y_{i+1} \mid Y^i, \boldsymbol{A}\big] &= \sum_{j=1}^{n} A_{ij}(X_j - \mathbb{E}\big[X_j \mid Y^i, \boldsymbol{A}\big]) + W_i \\ &\approx \mathcal{N}\left(0, \frac{1}{n} \operatorname{mmse}(\boldsymbol{X} \mid Y^i, \boldsymbol{A}) + \sigma^2\right) \end{aligned}$$

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- Hence,

$$I(\boldsymbol{X}, \boldsymbol{Y} \mid \boldsymbol{A}) \approx \sum_{i=0}^{m-1} \frac{1}{2} \log\left(1 + \frac{\frac{1}{n}\,\mathsf{mmse}(\boldsymbol{X} \mid Y^i, \boldsymbol{A})}{\sigma^2}\right)$$

Proof II: MMSE Satisfies Fixed-Point Equation

- By symmetry, MMSE is the same for all entries:

$$\frac{1}{n}\,\mathsf{mmse}(\boldsymbol{X} \mid \boldsymbol{Y}, \boldsymbol{A}) = \mathsf{mmse}(X_n \mid \boldsymbol{Y}, \boldsymbol{A})$$

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- If $p(\boldsymbol{x} \mid (Q\boldsymbol{Y})^{m-1}, \boldsymbol{A})$ is weakly correlated, then effective noise is approx. Gaussian and this leads to the fixed-point equation:

$$\mathsf{mmse}(X_n \mid \boldsymbol{Y}, \boldsymbol{A}) \approx M_X\left(\frac{m/n}{\sigma^2 + \frac{1}{n}\,\mathsf{mmse}(X^{n-1} \mid (Q\boldsymbol{Y})^m, \boldsymbol{A})}\right)$$

Proof III: Weak Correlation Almost Everywhere

- By chain rule and problem symmetry, we obtain:

$$I(\boldsymbol{X}; Y_{m+1} \mid Y^m, \boldsymbol{A}) = I(\boldsymbol{X}; Y_1 \mid \boldsymbol{A}) - \sum_{i=0}^{m-1} I(Y_{i+1}; Y_{i+2} \mid Y^i, \boldsymbol{A})$$

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$$\frac{1}{n^2} \sum_{k,\ell} \mathbb{E}\big[\mathsf{Cov}(X_k, X_\ell \mid Y^i, \boldsymbol{A})\big] \leq \Psi\big(I(Y_{i+1}; Y_{i+2} \mid Y^i, \boldsymbol{A})\big)$$

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- But $\sum_{i=0}^{\infty} I(Y_{i+1}; Y_{i+2} \mid Y^i, \boldsymbol{A}) \leq I(Y_1; \boldsymbol{X} \mid \boldsymbol{A})$ is finite, and thus

$$\#\{i : p(\boldsymbol{x} \mid Y^i, \boldsymbol{A}) \text{ has significant correlation}\} = o(n)$$

Proof IV: Resolve Limits via Area Theorem

Show that

$$\frac{1}{n} I(\boldsymbol{X}; \boldsymbol{Y} \mid \boldsymbol{A}) \approx \frac{1}{n} \sum_{i=1}^{m} \frac{1}{2} \log\left(1 + \frac{\frac{1}{n}\,\mathsf{mmse}(\boldsymbol{X} \mid Y^i, \boldsymbol{A})}{\sigma^2}\right)$$

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This implies asymptotic constraints

$$\mathcal{I}(\delta) = \int_0^\delta \frac{1}{2} \log\left(1 + \frac{\mathcal{E}(\delta')}{\sigma^2}\right) \mathrm{d}\delta' \qquad \text{integral constraint}$$

$$\mathcal{E}(\delta) = M_X\left(\frac{\delta}{\sigma^2 + \mathcal{E}(\delta)}\right), \quad \text{a.e.} \qquad \text{fixed-point constraint}$$

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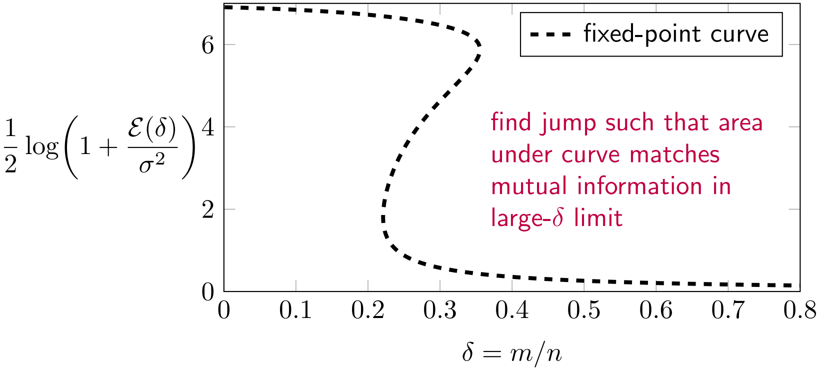

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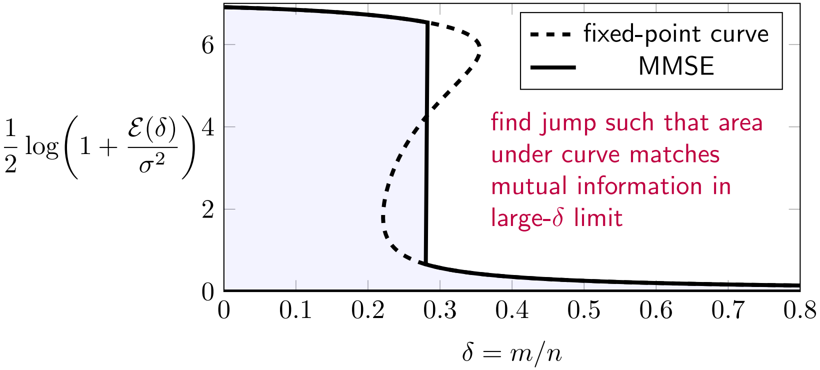

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Inference with Mismatched Prior

- Postulated distribution $q(\boldsymbol{x}, \boldsymbol{y})$ differs from true distribution $p(\boldsymbol{x}, \boldsymbol{y})$
- Example: MAP estimation via expectation with modified likelihood:

$$q_\beta(\boldsymbol{y}, \boldsymbol{x}) \propto [p(\boldsymbol{y} \mid \boldsymbol{x})]^\beta p(\boldsymbol{x})$$

$$\underbrace{\int \boldsymbol{x} q_\beta(\boldsymbol{x} \mid \boldsymbol{y})\, \mathrm{d}\boldsymbol{x}}_{\text{postulated mean}} \quad \xrightarrow{\beta \to \infty} \quad \underbrace{\arg\max_{\boldsymbol{x}} p(\boldsymbol{x} \mid \boldsymbol{y})}_{\text{MAP estimate}}$$

- Conjectured formulas for mismatched MMSE and M-estimators (e.g., MAP, MLE, LASSO)
- But replica symmetry does not hold in general!

Guo,Verdu'05, Rangan,Fletcher,Goyal'09, Bereyhi, Müller,Schulz-Baldes'17

Information in Multilayer Networks

Feed forward network with random weight matrices $\{W_\ell\}$

- Component-wise activation functions $\{\sigma_\ell\}$

$$\xrightarrow{\boldsymbol{x}} \boxed{\sigma_1(\boldsymbol{W}_1\boldsymbol{x})} \xrightarrow{\boldsymbol{h}_1} \cdots \xrightarrow{\boldsymbol{h}_{L-1}} \boxed{\sigma_L(\boldsymbol{W}_L\boldsymbol{h}_{L-1})} \xrightarrow{\boldsymbol{y}}$$

- Separable prior $p(\boldsymbol{x})$ and separable distributions $\{p_\ell(\cdot \mid \cdot)\}$

$$\boxed{p(\boldsymbol{x})} \xrightarrow{\boldsymbol{X}} \boxed{p_1(\cdot\,|\,\boldsymbol{W}_1\boldsymbol{x})} \xrightarrow{\boldsymbol{H}_1} \cdots \xrightarrow{\boldsymbol{H}_{L-1}} \boxed{p_L(\cdot\,|\,\boldsymbol{W}_L\boldsymbol{h}_{L-1})} \xrightarrow{\boldsymbol{Y}}$$

Manoel,Krzakala,Mézard,Zdeborová'17, Fletcher,Rangan,Schniter'18, R.'17, Gabrié,et.al'18

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What is mutual information between layers?

- State evolution for multilayer AMP / VAMP
- Conjectured formulas via heuristics
- Observed behavior under restricted learning of weights

Manoel,Krzakala,Mézard,Zdeborová'17, Fletcher,Rangan,Schniter'18, R.'17, Gabrié,et.al'18

Phase Diagrams in Other Problem

- Recent progress
  - Multilayer networks (random initialization)
  - Bilinear and multi-linear models (low rank) [See Jean's Talk]
  - Community detection (dense case)

Phase Diagrams in Other Problem

- Recent progress
  - Multilayer networks (random initialization)
  - Bilinear and multi-linear models (low rank) [See Jean's Talk]
  - Community detection (dense case)
- Future challenges
  - Multilayer networks (learned from data)
  - Bilinear and multi-linear models (extrinsic rank)
  - Community detection (sparse case)

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