Approximate Message Passing Tutorial

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NYU TANDON SCHOOL OF ENGINEERING

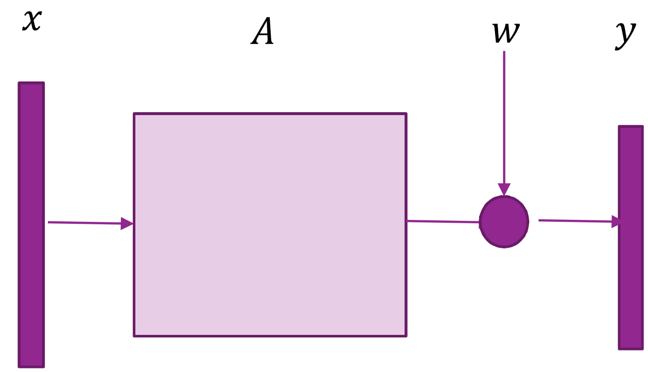
NYU WIRELESS

Outline

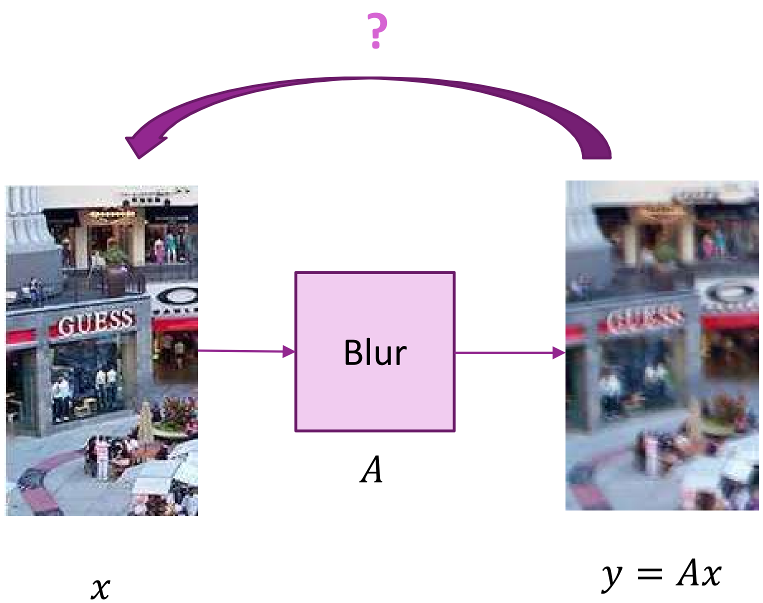
- AMP and Compressed Sensing
- Proximal Operators and ISTA
- State Evolution for AMP
- Bayes Denoising, Optimality and the Replica Method
- Belief Propagation and Factor Graphs
- AMP Derivation from Belief Propagation
- Convergence, Fixed Points and Stability
- Extensions: Vector AMP
- Thoughts on What is Next

Linear Inverse Problems

- Model:
$$y = Ax + w$$
  - x = unknown vector
  - w = "noise"
- Problem: Estimate x from A and y
- Many applications:
  - Linear regression with prior on weights
  - Compressed sensing
  - Image processing
  - …
- Will look at this problem and more complex variants



Example 1: Image Reconstruction



http://www.digitalphotopix.com/unbelievable/photo-deblur/
Article on Photoshop

- Recover original image x
- y = degraded / transformed image
- Operator A represents
  - Blurring
  - Measurement distortion
  - …
- Problem: Recover original x from y

Example 2: Multiple Linear Regression

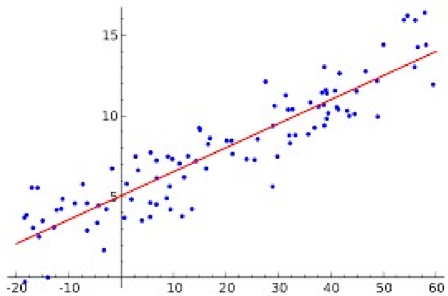
- Given data samples $(x_i, y_i), i = 1, \ldots, N$
  - Vector data: $x_i = (x_{i1}, \ldots, x_{id}), d =$number of features
- Problem: Fit a linear model

$$y_i = w_0 + w_1 x_{i1} + \cdots + w_d x_{id} + \epsilon_i$$

- Write in matrix form

$$y = Aw + \epsilon, \qquad A = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1d} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_{Nd} & \cdots & x_{Nd} \end{bmatrix}$$

- Estimate weight vector w from data



Unconstrained Least Squares Estimation

- Most common method for linear inverse problems is least squares estimation:

$$\hat{x} = \arg\min_{x} \frac{1}{2} \|y - Ax\|^2 = (A^T A)^{-1} A^T y$$

  - Computationally simple, easy to analyze, interpretable results
- Standard LS is unconstrained: Minimization above is all possible x
- But, in many problems, we have prior knowledge on x
  - Example: x is a natural image
- How do we incorporate prior knowledge?

Regularized Least Squares Estimation

- Regularized LS: Add a penalty term:

$$\hat{x} = \arg\min_x \frac{1}{2}\|y - Ax\|^2 + \phi(x)$$

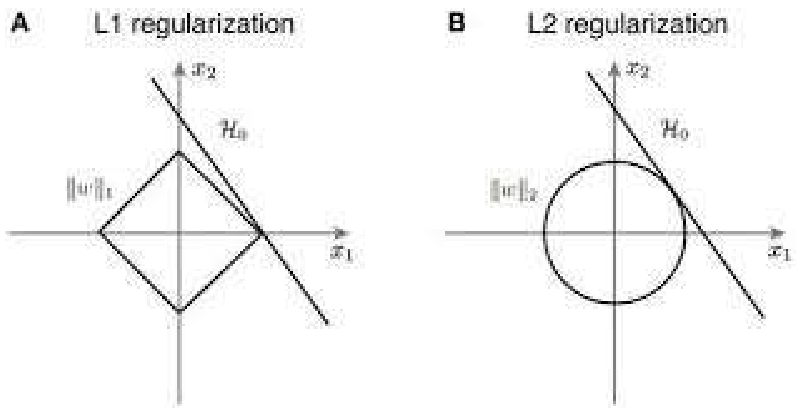
- $\phi(x)$ = Regularization function:
  - Penalizes values that are less likely or desirable as solutions
- Two common simple regularization functions:
  - L2 (called ridge regression in statistics): $\phi(x) = \lambda\|x\|_2^2 = \lambda\sum\left|x_j\right|^2$
  - L1 (called LASSO in statistics): $\phi(x) = \lambda\|x\|_1 = \lambda\sum|x_j|$
- Both functions force x to be close to zero (or some mean value if known)

L1 Regularization and Sparsity

- L1 regularized least-squares:

$$\hat{x} = \arg\min_{x} \frac{1}{2} \|y - Ax\|^2 + \lambda \|x\|_1$$

- L1 regularization favors sparse x
- Makes many coefficients exactly zero



L1 Regularization for Model Selection

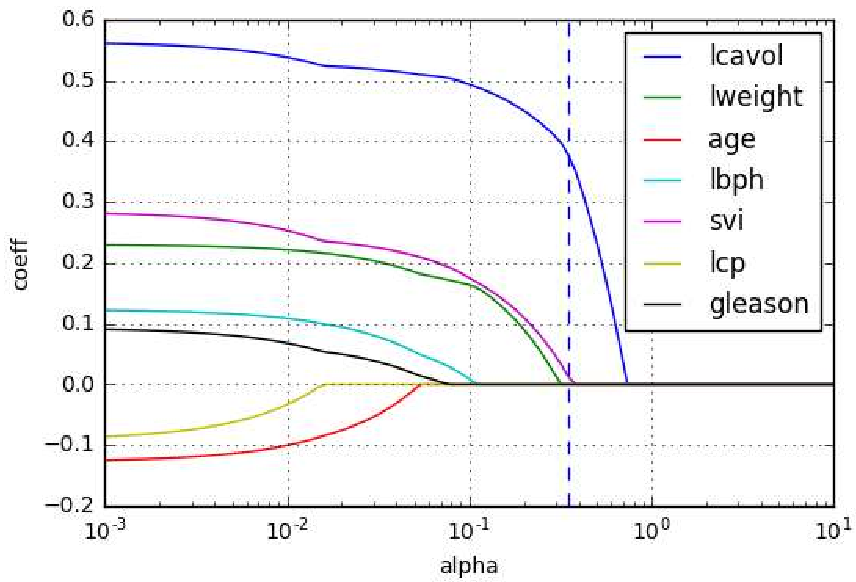
- Linear regression: Find weights w for

$$y_i = w_0 + w_1 x_{i1} + \cdots + w_d x_{id} + \epsilon_i$$

- Often need to perform model selection:
  - Number of features may be large
  - Only a few features are likely to be relevant
  - But, don't know which ones a priori
- Use LASSO estimation to find relevant features

$$\hat{w} = \arg\min_{x} \frac{1}{2}\|y - Aw\|^2 + \lambda \|w\|_1$$

  - Regularization tries to find a sparse weight vector
  - Many coefficients can be set to zero



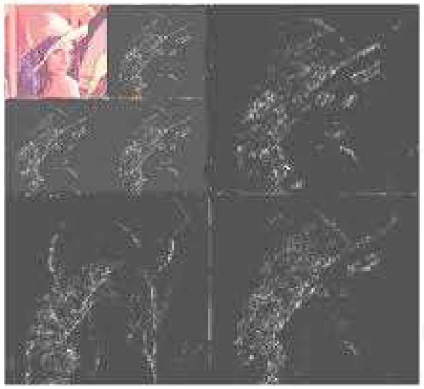
LASSO solutions for PSA level prediction
Path as a function of $\alpha = \lambda N$

L1 Estimation in Image Recovery

- Image x is often sparse in a transform domain
  - $u = Tx$ is sparse
  - Many transforms: Gradient operators, wavelet, …
  - All exploit that edges are sparse in natural images
- Use L1-regularization on transform components:

$$\hat{x} = \arg\min_{x} \frac{1}{2} \|y - Ax\|^2 + \lambda \|Tx\|_1$$

- Example: Total variation (TV) denoising
  - T= horizontal and vertical difference in pixels



Wavelet transform

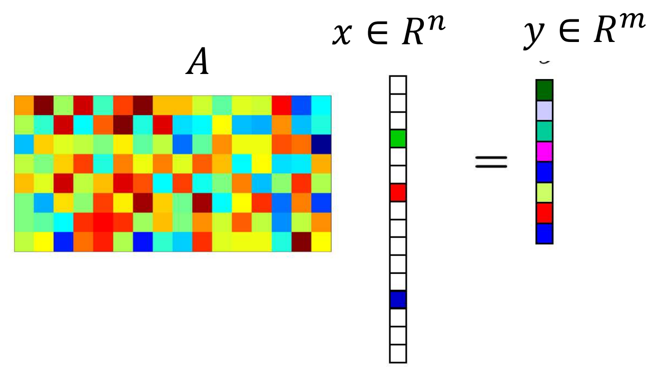
Transform is sparse

Compressed Sensing

- Revival of interest in L1 methods
  - [Donoho 06], [Candes, Romberg, Tao 06]
- Key observation:
  - Suppose x is sparse (e.g. $\|x\|_0 \leq k \ll n$)
  - Can recover x from underdetermined $y = Ax$
  - More unknowns than measurements (i.e. A is fat)
- Typical scaling of measurements:

$$m \geq Ck \log n$$

  - Requires incoherence of matrix with vector
  - Satisfied with random matrices with high probability



k non-zero elements

Compressed Sensing and its Challenges

- Significant work beginning 2006:
  - Scaling laws on measurements to recover “true” sparse vector
  - Fast algorithms
  - Successful applications, esp. in MRI

- Challenges:
  - Most analyses could only provide bounds. May be conservative.
  - Methods were often specific to L1 recovery. Difficult to generalized to other inverse problems
  - Hard to find theoretical optimal estimates
  - Ex: What is the minimum MSE: $E||\hat{x} - x_0||^2$ for a true vector x_0 with some noise model?
  - When can we achieve the optimal estimate and how?

Approximate Message Passing

- Benefits: For certain random matrices:
  - Very fast convergence
  - Can be precisely analyzed
  - Testable conditions for optimality
  - Can be extended to more complex models (parametric uncertainty, multilayer models, …)
- Problems / research questions: For general problems
  - Algorithm can diverge
  - Requires significant tuning
  - Requires precise specification of problem (partially solved)
- Arose out of study in compressed sensing
  - But, theory may provide insights to more complex models in inference today

AMP History

- Early work in CDMA detection for wireless
  - Boutros, Caire 02; Kabashima 02,03; Montanari & Tse (06), Guo & Wang (06), Tanaka & Okada (06)
- AMP re-discovered for compressed sensing
  - Donoho, Maleki, Montanari 09; Bayati-Montanari 10
- Connections to the replica method in statistical physics
  - Tanaka 04; Guo-Verdu 05;
  - Krzakala, F., Mézard, M., Sausset, F., Sun, Y. F., & Zdeborová, L. (2012)
  - Rangan, Fletcher, Goyal 09

AMP Extensions

- Since original paper, there have vast number of extensions
- GAMP: Generalized AMP for GLMs
- EM-(G)AMP: AMP with EM for parameter estimation
- BiGAMP: Bilinear AMP
- VAMP: Vector AMP that provides better convergence (end of this tutorial)
- ML-AMP and ML-VAMP: Multi-layer models
- Many more…

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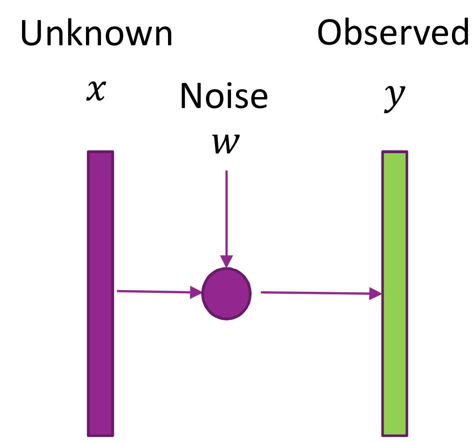
Proximal Operators

- Denoising problem: Given measurement $y = x + w$ estimate x
- Suppose we use a regularized estimator:

$$\hat{x} = \arg\min_x \frac{1}{2\tau}\|y - x\|^2 + \phi(x)$$

- Special case of regularized LS with $A = I$
  - We will look at adding general A matrix later
- The solution to this denoising problem is called the proximal operator

$$\text{Prox}_\phi(y,\tau) \coloneqq \arg\min_x \left[\frac{1}{2\tau}\|x - y\|^2 + \phi(x)\right]$$



Ex 1: Projections

- Proximal operators are generalizations of projections
- Suppose for some set C:

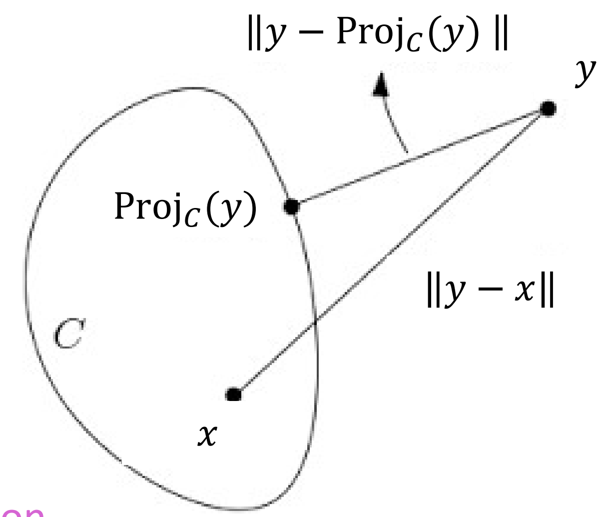
$$\phi(x) = \begin{cases} 0 & x \in C \\ \infty & x \notin C \end{cases}$$

- Then, proximal operator is a projection

$$\mathrm{Prox}_\phi(y,\tau) := \arg\min_x \left[\phi(x) + \frac{1}{2\tau}\|x-y\|^2\right]$$

$$= \arg\min_{x\in C}\|x-y\|^2 = \mathrm{Proj}_C(y)$$

- For general $\phi(\cdot)$, proximal operator $\mathrm{Prox}_\phi(y,\tau)$ is a "soft" projection
  - Finds points close to y where $\phi(x)$ is small



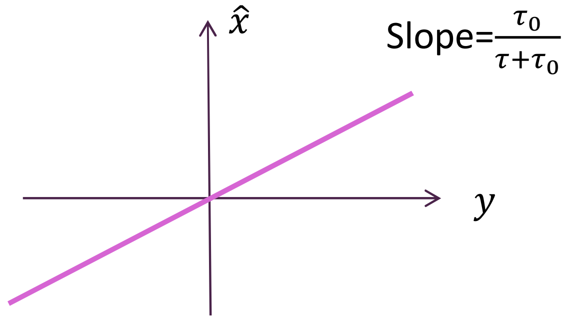
Ex 2: Scalar L2 / Quadratic Penalty

- Consider a quadratic penalty $\phi(x) := \frac{1}{2\tau_0}(x - x_0)^2$
  - Denoising is equivalent to a Gaussian prior
- Then, proximal operator is a linear function:

$$\text{Prox}_\phi(y,\tau) := \arg\min_x \left[\phi(x) + \frac{1}{2\tau}(x-y)^2\right]$$
$$= \frac{1}{\tau+\tau_0}[\tau x_0 + \tau_0 y]$$

  - Convex combination of observed y and prior x_0
- When $x_0 = 0$, get a shrinkage to zero:

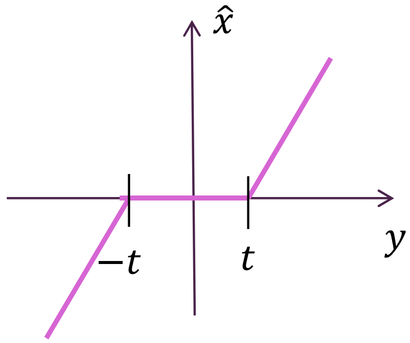
$$\text{Prox}_\phi(y,\tau) = \frac{\tau_0}{\tau+\tau_0} y$$



Ex 3: Scalar L1 Penalty

- L1 penalty: $\phi(x) = \lambda|x|$
  - Scalar LASSO problem
- Proximal operator is a soft-threshold

$$\mathrm{Prox}_\phi(y,\tau) = \begin{cases} y - t & y > t \\ 0 & |y| \le t \\ y + t & y < -t \end{cases}, \qquad t = \tau\lambda$$



- Can result in exactly zero solutions

Ex 4: Separable Penalties

- Suppose $\phi(x)$ is separable:

$$\phi(x) = \sum_{i=1}^{N} \phi_i(x_i)$$

- Example: L1 and L2 penalties
  - $\phi(x) = \|x\|_2^2 = \sum |x_i|^2$
  - $\phi(x) = \|x\|_1 = \sum |x_i|$
- Then, proximal operator applies componentwise

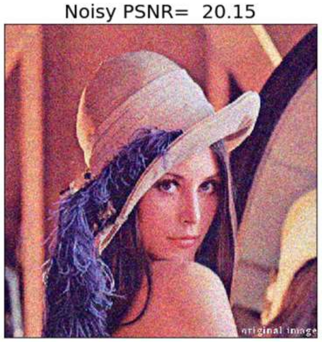
$$\hat{x} = \mathrm{Prox}_{\phi}(y, \tau) \Leftrightarrow \hat{x}_i = \mathrm{Prox}_{\phi_i}(y_i, \tau)$$

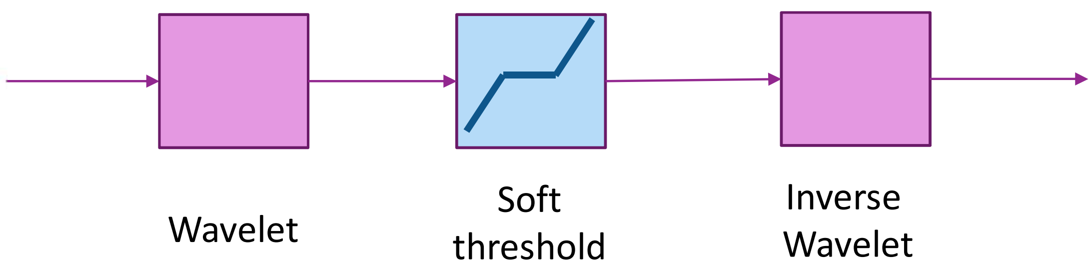
  - Apply proximal operator on each component

Ex 5: Wavelet Image Soft-Thresholding

- Suppose penalty is applied in wavelet domain: $\phi(x) = h(Wx)$,
  - W = orthogonal wavelet transform
- Often use L1 penalty: $h(z) = \begin{cases} 0 & \text{if } z_n \text{ is a scale coefficient} \\ \lambda|z_n| & \text{if } z_n \text{ is a detail coefficient} \end{cases}$
- Proximal operator can be applied in wavelet domain: $\mathrm{Prox}_\phi(y,\tau) = W^{-1}\mathrm{Prox}_h(Wy,\tau)$
  - Use fact that W is orthogonal

Noisy PSNR= 20.15





Soft-Thresh PSNR= 27.35

Regularized LS Estimation

- Now, return to regularized LS problem:

$$\hat{x} = \arg\min_x \frac{1}{2}\|y - Ax\|^2 + \phi(x)$$

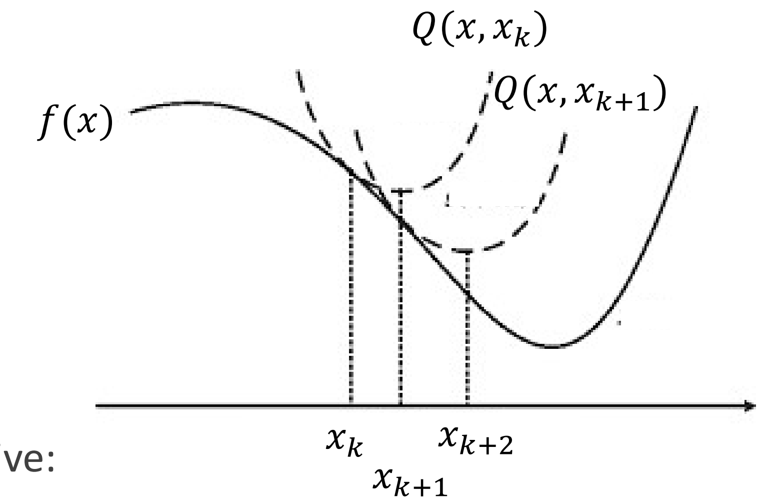
  - For LASSO: $\phi(x) = \lambda\|x\|_1$

- Challenges:
  - No closed form solution when $A \neq I$
  - Objective is non-smooth
  - Cannot directly apply gradient descent

- ISTA: Iterative Soft Thresholding Algorithm
  - Key idea: Break problems into sequence of proximal problems
  - Based on majorization minimization (next slide)

Majorization-Minimization

- Suppose minimizing $f(x)$ is hard to minimize directly
- At each x_k, find a majorizing function $Q(x, x_k)$:
  - $Q(x, x_k) \geq f(x)$ for all x
  - $Q(x_k, x_k) = f(x_k)$
- Majorization-Minimization algorithm:
  Iteratively minimize the majorizing function:
  $$x_{k+1} = \arg\min_{x} Q(x, x_k)$$
- Theorem: MM monotonically decreases the true objective:
  $$f(x_k) = Q(x_k, x_k) \geq Q(x_{k+1}, x_k) \geq f(x_{k+1})$$



MM for Regularized LS

- Rewrite regularized LS with two components:

$$\hat{x} = \arg\min_{x}[g(x) + \phi(x)]$$

  - Smooth component: $g(x) \coloneqq \frac{1}{2}\|y - Ax\|^2$
  - Non-smooth but separable component: $\phi(x) = \lambda\|x\|_1$

- Define majorizing function:

$$Q(x, x_k) \coloneqq g(x_k) + \nabla g(x_k) \cdot (x - x_k) + \frac{1}{2\alpha}\|x - x_k\|^2 + \phi(x)$$

- Easy to verify two properties:
  - $Q(x_k, x_k) = g(x_k) + h(x_k) = f(x_k)$
  - If α is sufficiently small, $Q(x, x_k) \geq F(x_k)$ for all x

- MM Algorithm:

$$x_{k+1} = \arg\min_{x} Q(x, x_k) = \arg\min_{x}\left[\phi(x) + \nabla g(x_k) \cdot (x - x_k) + \frac{1}{2\alpha}\|x - x_k\|^2\right]$$

ISTA Algorithm

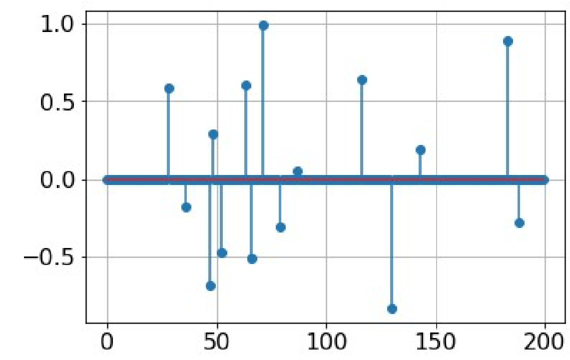
- From previous slide, MM algorithm is:

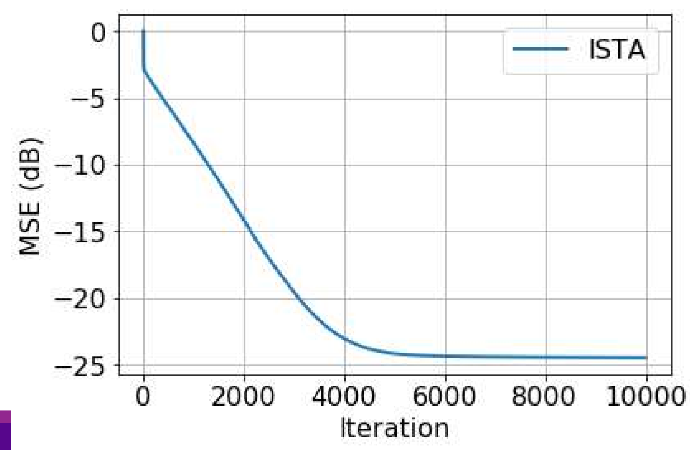
$$x_{k+1} = \arg\min_x Q(x, x_k) = \arg\min_x \left[\phi(x) + \nabla g(x_k) \cdot (x - x_k) + \frac{1}{2\alpha}\|x - x_k\|^2\right]$$

- Completing squares of MM Algorithm, we obtain two step algorithm
- Iterative Soft Threshold Algorithm:
  - Gradient step: $r_k = x_k - \alpha \nabla g(x_k) = r_k - \alpha A^T(Ax_k - y)$
  - Proximal step: $x_{k+1} = \mathrm{Prox}_\phi(r_k, \alpha)$
- Estimation is performed by sequence of proximal operators
  - For L1 / LASSO minimization, proximal operators are soft thresholds

Simple Compressed Sensing Example

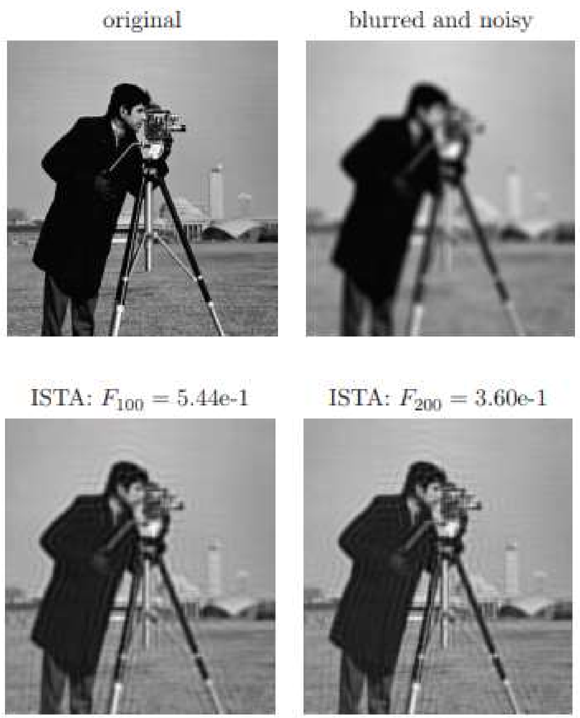
- Synthetic sparse signal:
  - $x_i = \begin{cases} 0 & \text{with prob } 1-\rho = 0.9 \\ N(0,1) & \text{with prob } \rho = 0.1 \end{cases}$
- Random measurement matrix $A \in R^{100\times200}$
  - $A_{ij} \sim N\left(0, \frac{1}{N}\right), \; N = 200$
  - Underdetermined
  - SNR = 30 dB noise
- Use LASSO estimate with $\lambda = 10$





Wavelet Image Deblurring with ISTA

- Measurements: $y = Ax + w$
  - $A =$ Gaussian blur
  - $w =$ Gaussian noise
- Denoiser uses 3 level Haar wavelet
- Decent results after 200 iterations



Beck, Amir, and Marc Teboulle. "A fast iterative shrinkage-thresholding algorithm for linear inverse problems." *SIAM journal on imaging sciences* 2.1 (2009): 183-202.

ADMM

- Proximal operators also appear in Alternating Direction Method of Multipliers (ADMM)
- Consider cost function: $f(x) = g(x) + h(x)$
- Variable splitting: Equivalent constrained minimization:

$$\min_{x,y} g(x) + h(y) \quad s.t.\ x = y$$

- Define augmented Lagrangian:

$$L(x, y, s) \coloneqq g(x) + h(y) + \alpha s^T(x - y) + \frac{\alpha}{2}\|x - y\|^2$$

- ADMM algorithm:
  - $\hat{x} = \arg\min_x L(x, \hat{y}, s)$
  - $\hat{y} = \arg\min_y L(\hat{x}, y, s)$
  - $s = s + x - y$

ADMM with Proximal Operators

- Complete squares as before
- ADMM can be rewritten with two proximal operators
  - $\hat{x} = \arg\min_x L(x, \hat{y}, s) = \mathrm{Prox}_g(\hat{y} - s; \alpha^{-1})$
  - $\hat{y} = \arg\min_y L(\hat{x}, y, s) = \mathrm{Prox}_h(\hat{x} + s; \alpha^{-1})$
  - $s = s + x - y$
- For LASSO problem:
  - $g(x) \coloneqq \frac{1}{2}\|b - Ax\|^2 \Rightarrow \mathrm{Prox}_g(u; \alpha^{-1}) = (A^T A + \alpha I)^{-1}(A^T b + \alpha u)$
  - $h(y) \coloneqq \lambda\|y\|_1 \Rightarrow \mathrm{Prox}_h(u; \alpha^{-1}) = T_t(u)$

Questions

- Proximal operator methods can guarantee convergence to a local minima
  - Appears to work in well in several key problems, esp. L1 regularized LS
  - Can be applied to non-smooth optimization
- Tremendous additional work (not covered here)
  - Rates of convergence
  - Interesting denoisers (low rank matrix recovery)
  - …
- But, several open questions:
  - How close are the resulting solutions to the correct value?
  - What is the “optimal” estimate?
  - Can we converge faster?
  - Describe this more…

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ISTA

- Consider regularized LS problem:

$$\hat{x} = \arg\min_x \left[\frac{1}{2}\|y - Ax\|^2 + \phi(x)\right]$$

  - For LASSO, $\phi(x) = \lambda_1 \|x\|_1$

- ISTA algorithm from previous section:
  - $d_k = y - A\hat{x}_k$
  - $r_k = \hat{x}_k + \tau A^T d_k$
  - $\hat{x}_{k+1} = \text{Prox}_\phi(r_k, \tau)$

- Can we do better?

Approximate Message Passing

AMP

$$d_k = y - A\hat{x}_k + \frac{N}{M}\alpha_k d_{k-1}$$

$$r_k = \hat{x}_k + A^T d_k$$

$$\hat{x}_{k+1} = g_{in}(r_k, \theta^k)$$

$$\alpha_{k+1} = \langle g'_{in}(r_k, \theta^k)\rangle = \frac{1}{N}\sum_i \frac{\partial g_{in}(r_k, \theta^k)}{\partial r_{ki}}$$

Note: A and y must be scaled such that:

$$||A||_F^2 = N$$

ISTA

$$d_k = y - A\hat{x}_k$$
$$r_k = \hat{x}_k + \tau A^T d_k$$
$$\hat{x}_{k+1} = \mathrm{Prox}_\phi(r_k, \tau)$$

Key modifications for AMP

- Memory term in the residual update $\alpha_k d_{k-1}$
  - Acts as a momentum
  - Called the “Onsager term” in statistical physics
  - More on this soon
- Proximal operator replaced by general estimator
  - θ^k is an arbitrary parameter of the estimator

Fixed Points

- Theorem: At any fixed point of AMP with a proximal denoiser $\hat{x} = \mathrm{Prox}_{\phi}(r,\tau)$

$$\hat{x} = \arg\min_{x}[\lambda\phi(x) + g(x)], \qquad g(x) = \frac{1}{2}\|y - Ax\|^2, \qquad \lambda = (1-\alpha)\tau$$

- Proof: For any fixed point:
  - $d = y - A\hat{x} + \alpha d \Rightarrow d = \frac{y - A\hat{x}}{1-\alpha}$
  - $r = \hat{x} + A^T d = \hat{x} - \frac{1}{1-\alpha}\nabla g(\hat{x})$

- If we use a proximal denoiser: $\hat{x} = \mathrm{Prox}_{\phi}(r,\tau)$

$$\begin{aligned}\hat{x} &= \arg\min_{x}\left[\phi(x) + \frac{1}{2\tau}\|r - x\|^2\right] \\ &= \arg\min_{x}\left[\phi(x) + \frac{1}{(1-\alpha)\tau}\nabla g(\hat{x})^T(x - \hat{x}) + \frac{1}{2\tau}\|\hat{x} - x\|^2\right]\end{aligned}$$

Selecting the AMP step size

- AMP "solves" the regularized LS problem (when it converges):

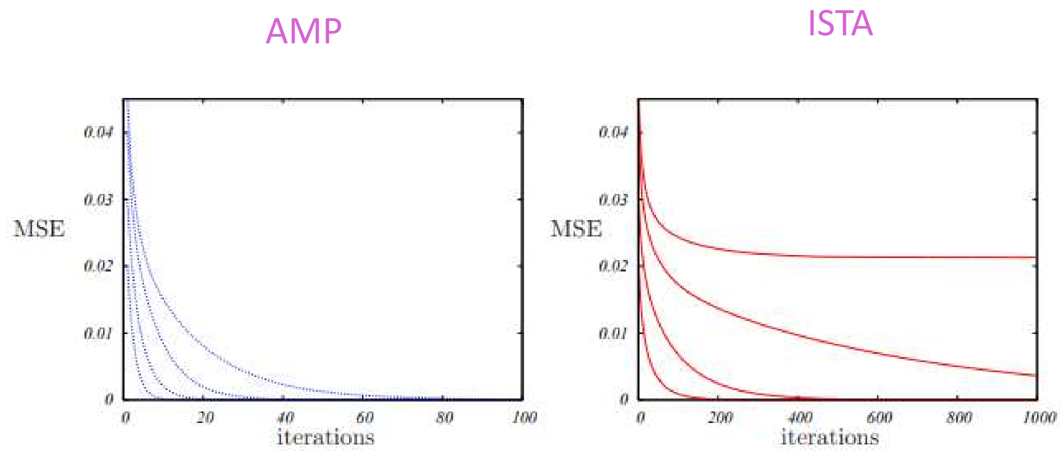
$$\hat{x} = \arg\min_x \left[\lambda\phi(x) + \frac{1}{2}\|y - Ax\|^2 \right]$$

- But, regularization parameter is computed implicitly: $\lambda = (1-\alpha)\theta$
- For LASSO problem:
  - Typically select threshold directly $t = c\frac{\|d_k\|}{\sqrt{N}}$ for some constant c
  - Constant c is larger when sparsity is greater
  - Tune c instead of λ

Compressed Sensing Example

- Sparse random vector example
  - $N = 8000, M = 1600$
  - $\|x\|_0 = \{800,1200,1600,1800\}$
  - $A_{ij} \sim N(0, \frac{1}{M})$

- AMP: Much faster convergence
  - Look at axes!



Montanari, "Graphical models concepts in compressed sensing." *Compressed Sensing: Theory and Applications* (2012)

Large System Limit

- When does AMP work so well? Why?
- Analysis of AMP is generally in a large system limit
- Sequence of problems $N \to \infty$ with $\lim_{N\to\infty} \frac{M}{N} = \beta$
- Assumptions: For every N:
  - There is a true vector x_0 and noise w with $y = Ax_0 + w$
  - Random matrix: $A \in R^{M\times N}$, $A_{ij} \sim N\left(0, \frac{1}{M}\right)$
  - Estimator $g(r,\tau)$ is Lipschitz in r and acts componentwise: $g(r,\tau)_i = g(r_i,\tau)$
  - Vectors x_0, $\hat{x}_j^0$ and w are i.i.d. and independent of A: $x_{0j} \sim X_0$, $w_i \sim W$, $\hat{x}_j^0 \sim \hat{X}^0$
- Note that due to normalization: $||A||_F^2 \approx N$

Scalar MSE Function

- Want to predict the asymptotic MSE in each iteration:

$$\eta^k := \lim_{N \to \infty} \frac{1}{N} \left\| \hat{x}^k - x_0 \right\|^2$$

- Define the scalar MSE function:

$$MSE(\nu, \theta) := E|g(X_0 + N(0, \nu), \theta) - X_0|^2,$$

  - Average error on a single component of the estimate $\hat{X} = g(R, \theta)$ with $R = X_0 + N(0, \nu)$
  - Estimation error under Gaussian noise

- Can be computed via scalar integrals $\Rightarrow$ Easy!
- We will show: $\eta^k = MSE(\nu^k, \theta^k)$ where ν^k can be computed recursively

Ex 1: MSE Function for an L2 Penalty

- Suppose that estimator is linear: $g(r,\theta) = \theta r$
  - Proximal estimator corresponding to a L2 / quadratic penalty
- Then MSE is given by:

$$\begin{aligned}\text{MSE}(\nu,\theta) &= E|g(X_0 + N(0,\nu),\theta) - X_0|^2 \\ &= E|\theta(X_0 + V) - X_0|^2 = (1-\theta)^2 E|X_0|^2 + \theta^2 \nu\end{aligned}$$

- If $E|X_0|^2$ and ν were known, we could optimize θ:

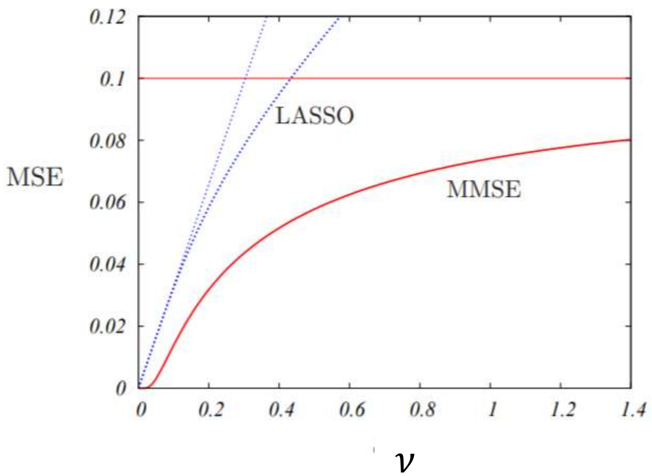
$$\hat{\theta} = \frac{E|X_0|^2}{E|X_0|^2 + \nu}, \qquad \min_{\theta} MSE\ (\nu,\theta) = \frac{\nu E|X_0|^2}{E|X_0|^2 + \nu}$$

  - Called the linear minimum MSE estimator (LMMSE) in signal processing

Ex 2: MSE Function for an L1 Penalty

- Suppose true signal is 3-point sparse $\mathrm{P}(X_0 = x) = \begin{cases} \rho/2 & x = 1 \\ 1-\rho & x = 0 \\ \rho/2 & x = -1 \end{cases}$ $\rho = 0.1$

- Two estimators:
  - LASSO with optimized λ
  - MMSE: $\hat{X} = \mathrm{E}(\mathrm{X}_0 | \mathrm{R} = \mathrm{X}_0 + \mathrm{N}(0, \nu))$



Montanari, "Graphical models concepts in compressed sensing." *Compressed Sensing: Theory and Applications* (2012)

State Evolution

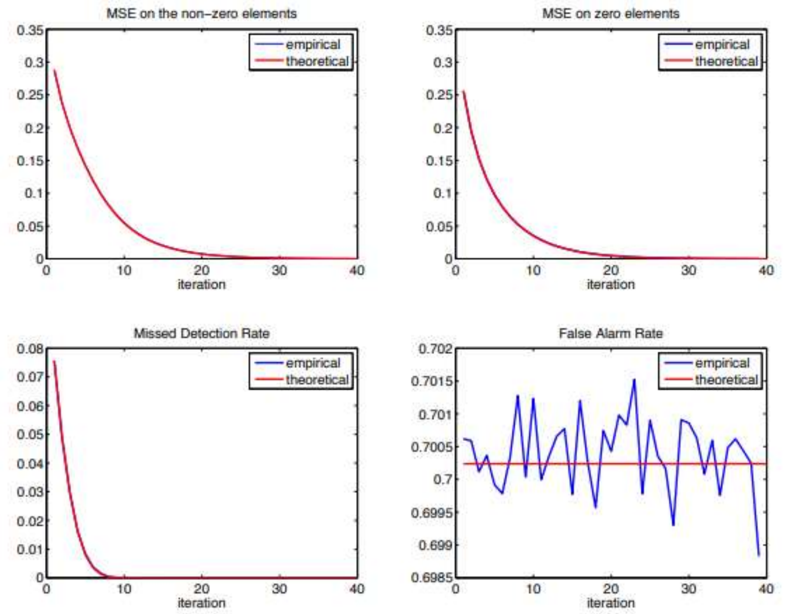
- Theorem: In the large system limit, the asymptotic MSE evolves as:

$$\eta^{k+1} = MSE\left(\frac{N}{M}\eta^k + E|W|^2, \theta^k\right), \qquad \eta^0 = E\left|\hat{X}^0 - X_0\right|^2$$

- In the LSL, MSE can be exactly predicted!
- Result is very general:
  - All i.i.d. densities on the true signal x_0
  - Separable Lipschitz estimators $\hat{x}^k = g(r^k, \theta^k)$ with any parameters θ^k
  - Can account for estimators of non-convex functions

State Evolution Example 1

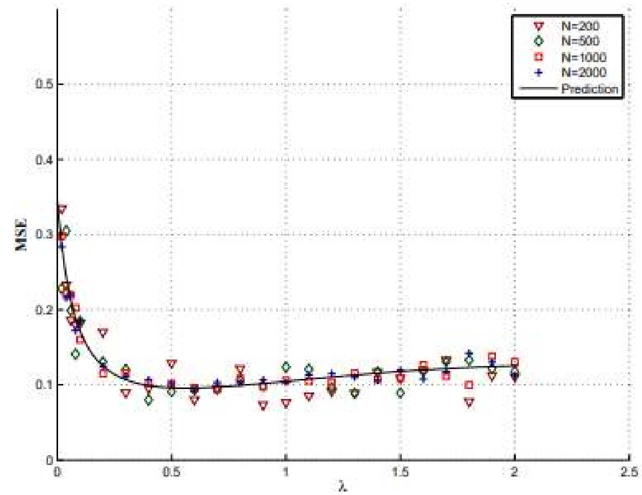
- Can predict the MSE per component exactly!
- Can also predict various statistics
  - eg. Missed detection, false alarm rate
  - Will show how to do this later
- Simulation parameters:
  - $x_{0j} = \begin{cases} 1 & \text{Prob} = \rho \\ 0 & \text{Prob} = 1-\rho \end{cases}, \ \rho = 0.045$
  - $N = 5000, \frac{\mathrm{M}}{N} = 0.3$
  - No noise



Donoho, Maleki, Montanari. "Message passing algorithms for compressed sensing: I. motivation and construction." *ITW 2010*

State Evolution Example 2

- Comparison of predicted limit of SE
  - Predicted = $\lim_{k\to\infty} \eta^k$
  - Simulated = measured MSE
- We obtain close to an exact match
  - Match improves as N increases
- Simulation parameters
  - x iid three point density
  - N varies, $\frac{M}{N} = 0.64$



Error Vectors

- Proof of the SE requires that we track certain error quantities
- AMP algorithm:
  - $d_k = y - A\hat{x}_k + \frac{N}{M}\alpha_k d_{k-1}$
  - $r_k = \hat{x}_k + A^T d_k$
  - $\hat{x}_{k+1} = g_{in}(r_k, \theta^k), \;\; \alpha_{k+1} = \langle g'_{in}(r_k, \theta^k) \rangle$
- Define the error vectors:
  - $u^k = \hat{x}^k - x_0$: Error after estimator
  - $q^k = r^k - x_0$: : Error before estimator
  - $v^k = d^k$: Output error with noise
  - $p^k = d^k - w = A(\hat{x}^k - x_0) - \alpha^k d^{k-1}$: Output prediction without noise
- Scalar error functions:
  - Output: $G_p(p, w, \tau) \coloneqq w - p$
  - Input: $G_q(q, w, \tau) \coloneqq g(q + x_0, \tau) - x_0$

Error System

- Simple algebra shows that error vectors evolve as the general recursion:
  - $p^k = Au^k - \lambda_u^k v^{k-1}$
  - $v^k = G_p(p^k, w_p, \theta_p^k),\ \lambda_v^k = \langle G_p'(p^k, w_p, \theta_p^k)\rangle$
  - $q^k = A^T v^k - \lambda_v^k u^k$
  - $u^{k+1} = G_q(q^k, w_q, \theta_q^k), \quad \lambda_u^k = \langle G_q'(q^k, w_q, \theta_q^k)\rangle$

- Simple structure: Each iteration involves:
  - Multiplication by A and A^T
  - Componentwise nonlinearities

Main Result: Scalar Equivalence

Error system:

- $p^k = Au^k - \lambda_u^k v^{k-1}$,
- $v^k = G_p\left(p^k, w_p, \theta_p^k\right)$, $\lambda_v^k = \left\langle G_p'\left(p^k, w_p, \theta_p^k\right)\right\rangle$
- $q^k = A^T v^k - \lambda_v^k u^k$,
- $u^{k+1} = G_q\left(q^k, w_q, \theta_q^k\right)$, $\lambda_u^k = \left\langle G_q'\left(q^k, w_q, \theta_q^k\right)\right\rangle$

=

Scalar system

- $P^k \sim N\left(0, \tau_p^k\right)$, $\tau_p^k = \frac{N}{M} E\left|U^k\right|^2$
- $V^k = G_p(P^k, W_p, \theta_p^k)$
- $Q^k \sim N\left(0, \tau_q^k\right)$, $\tau_q^k = E\left|V^k\right|^2$
- $U^{k+1} = G_q(Q^k, W_q, \theta_q^k)$

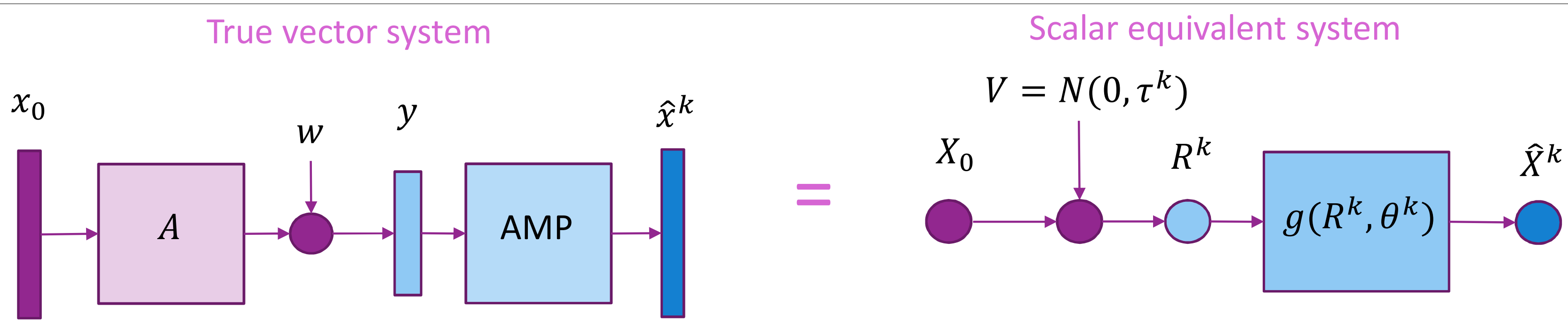
❑ Theorem [Bayati-Montanari 2010]: In the large system limit:

- Distribution of components error system vectors = distribution of scalar random variables

$$\lim_{N\to\infty} p^k = P^k, \lim_{N\to\infty} q^k = Q^k, \ldots$$

- Formal definition of convergence given below
- Shows errors are Gaussian
- AMP SE follows as special case

Scalar Equivalent Model



- ❑Each component of the vector system behaves like a simple scalar model
- ❑Equivalent to estimating component in Gaussian noise
- ❑Level of Gaussian noise accounts for "interference" between components from A
- ❑Also called a decoupling principle or single letter model

Convergence Formalities

- In what sense do vectors "converge empirically" in Bayati-Monanari result?
- Consider a sequence of vectors $x = x(N) \in R^N$
  - Dimension of vector grows with N. Vector can be deterministic
- Definition: A function $\phi \in PL(k)$ if:
$$\|\phi(x) - \phi(y)\| \leq L\|x - y\|\left[1 + \|x - y\|^{k-1}\right]$$
  - For $k = 1$, this is the standard Lipschitz continuity
- Definition: Sequence $x = x(N)$ converges empirically $PL(k)$ to a scalar X if:
$$\lim_{N\to\infty} \frac{1}{N} \sum\nolimits_n \phi(x_n) = E\big(\phi(X)\big) < \infty \text{ for all } \phi \in PL(k)$$
  - Satisfied for $x_n \sim X$ i.i.d. if $E|X|^k < \infty$

Metrics

- Scalar equivalent model can be used to measure any separable metric
- Ex: MSE. Take $\phi(x_0, \hat{x}^k) := \left|\hat{x}^k - x_0\right|^2$. Then,

$$\text{MSE} = \frac{1}{N}\left\|x_0 - \hat{x}^k\right\|^2 = \frac{1}{N}\sum_{j=1}^{N}\phi(x_{0j}, \hat{x}_j^k) = E\phi\left(X_0, \hat{X}^k\right) = \left|\hat{X}^k - X_0\right|^2$$

- Can also other separable metrics:
  - False alarm, missed detection
  - Error thresholds …

Proof of SE: First Half Iteration

- For $k = 0$: $p^0 = Au^0$

$$p_i^0 = \sum_{j=1}^{N} A_{ij} u_j^0$$

- Since A is i.i.d. $A_{ij} = N(0, \frac{1}{M})$, and u_j^0 are i.i.d. independent of one another:

$$p_i^0 \to N\left(0, \frac{N}{M} E|U^0|^2\right)$$

- Components are Gaussian
- But, this argument doesn't work for $k > 0$
  - A_{ij} becomes dependent on u_j^k

Intuition for $k > 0$. Part I

- Now consider subsequent iteration:

$$q_j^k = \sum_{i=1}^{M} A_{ij} G_q(p_i^k, w_{pi}) - \lambda_u^k u_j^k, \qquad p_i^k = \sum A_{i\ell}\, u_\ell^k$$

- Problems for analysis:
  - Variables are no longer independent
- Idea: Remove dependence between A_{ij} and $A_{ij} u_j^k$
- Define $p_{i\backslash j}^k = p_i^k - A_{ij} u_j^k = \sum_{\ell \neq j} A_{i\ell}\, u_\ell^k$
- Then:

$$q_j^k \approx \sum_{i=1}^{M} \left[A_{ij} G_q\left(p_{i\backslash j}^k, w_{pi}\right) + A_{ij}^2 u_j^k G_q'(p_{i\backslash j}, w_{pi}) \right] - \lambda_u^k u_j^k$$

Intuition for $k > 0$. Part 2

- From before: $q_j^k \approx \sum_{i=1}^{M} \left[A_{ij} G_p\left(p_{i\backslash j}^k, w_{pi}\right) + A_{ij}^2 u_j^k G_p'(p_{i\backslash j}, w_{pi}) \right] - \lambda_u^k u_j^k$
- Now assume A_{ij} is independent of $p_{i\backslash j}^k$
  - We have subtracted the term $A_{ij} u_j^k$
- Since $A_{ij} = N(0, \frac{1}{M})$:

$$\sum_i A_{ij}^2 G_p'(p_{i\backslash j}, w_{pi}) \approx \frac{1}{M} \sum_i G_q'\left(p_{i\backslash j}, w_{pi}\right) \approx \frac{1}{M} \sum_i G_q'\left(p_i, w_{pi}\right) = \lambda_u^k$$

- Also, by CLT: $\sum_i A_{ij} G_q\left(p_{i\backslash j}^k, w_{pi}\right) \approx N\left(0, \tau_q^k\right)$

$$\tau_p^k = \frac{1}{M} \sum_i G_p^2\left(p_{i\backslash j}, w_{pi}\right) \approx \frac{1}{M} \sum_i G_p^2\left(p_i^k, w_{pi}\right) = E G_p^2\left(P^k, W_p\right)$$

Bolthausen Conditioning 1

- How do we make above argument rigorous?
- Key idea of Bayati-Montanari 10
  - Credited to Erwin Bolthausen 14
- Consider conditional distribution of A after k iterations
- After k iterations, we know:

$$p^j = Au^j - \lambda_u^j v^{j-1}, \qquad q^j = A^T v^j - \lambda_u^j u^j, \qquad j = 0,1,\ldots,k$$

- Each iteration reveals actions on vectors u^k and v^k

Bolthausen Conditioning 2

- Want the conditional distribution of A subject to linear constraints
  - $X = AU, \quad U = \left[u^0\, u^1 \cdots u^k\right], \quad X = [p^0, p^1 + \lambda_v^0 u^0, \cdots, p^k + \lambda_v^{k-1} u^{k-1}]$
  - $Y = A^T V, \quad V = \left[v^0\, v^1 \cdots v^k\right], \quad Y = [q^0, q^1 + \lambda_u^0 v^0, \cdots, q^{k-1} + \lambda_u^{k-2} v^{k-2}]$
- This is just conditional distribution of a Gaussian subject to linear constraints
- Can show, conditional distribution is:

$$A = E + P_V^{\perp}\, \tilde{A} P_U^{\perp}$$

  - E is a deterministic matrix with from U, X, V, Y
  - $P_U^{\perp}, P_V^{\perp}$ are projection operators
  - $\tilde{A}$ is independent of U, X, V, Y

Bolthausen Conditioning 3

- We have $A = E + P_V^{\perp}\,\tilde{A}P_U^{\perp}$
- Consider action: $Av^k = Ev^k + P_V^{\perp}\,\tilde{A}P_U^{\perp}v^k$
- Second term: $P_V^{\perp}\,\tilde{A}P_U^{\perp}v^k \approx \tilde{A}v^k$= i.i.d. Gaussian
  - Uses independence of $\tilde{A}$
  - Projections remove only k of N components. So, their effect is small as $N \to \infty$
- First term: Ev^k
  - Can write in terms of inner products $\langle p^j, v^k \rangle = \frac{1}{M}\sum_i p_i^j\, v_i^k = \frac{1}{M}\sum_i p_i^j\, G_p(p_i^j, w_{pi})$
  - Induction hypothesis: $\langle p^j, v^k \rangle = E\left(P^j G_p(P^k, W_p)\right)$
  - By Gaussianity and Stein's Lemma: $\langle p^j, v^k \rangle = E\left(G_p'(P^k, W_p)\right) E(P^j P^k)$
  - With lots of algebra, this shows: : $Ev^k \approx \lambda_u^k \mathrm{u}^{k-1}$

Outline

- AMP and Compressed Sensing
- Proximal Operators and ISTA
- State Evolution for AMP
- Bayes Denoising, Optimality and the Replica Method
- Belief Propagation and Factor Graphs
- AMP Derivation from Belief Propagation
- Convergence, Fixed Points and Stability
- Extensions: Vector AMP
- Thoughts on What is Next

Optimizing the MSE

- SE shows: $\eta^{k+1} = MSE\left(\frac{N}{M}\eta^k + E|W|^2, \theta^k\right)$
- MSE function depends on the estimator:
$$MSE(\nu, \theta) \coloneqq E|g(X_0 + N(0,\nu), \theta) - X_0|^2$$
- Suppose that distribution on X_0 is known
  - Equivalent to known the statistics on the unknown vector exactly
- Idea: Select $g(\cdot)$ to minimize the MSE.
- Optimal estimator is: $g(r) = E(X_0 | R = r,\ R = X_0 + N(0,\nu))$
- Minimum MSE is:
$$MSE^*(\nu) \coloneqq Var(X_0 | X_0 + N(0,\nu))$$

Implementing the MMSE Estimator

- Implementation is possible if:
  - x_0 is well-modeled as i.i.d. and
  - Distribution of components $x_{0j} \sim X_0$ is known
- MMSE estimator can often be analytically for many densities
  - Ex: X_0 is a Gaussian-Mixture Model (GMM):

$$p(X_0|Z=i) = N(\mu_i, \tau_i), \qquad P(Z=i) = q_i, \qquad i = 1,..,L$$

  - Then

$$g(r) = E(X_0|R = X_0 + N(0,v)) = \sum_i E(X_0|R, Z=i)P(Z=i|R)$$

- General densities can be done with numerical integration
  - Or some approximation

Optimality

- With MMSE estimator, SE is: $\eta^{k+1} = MSE^*\left(\frac{N}{M}\eta^k + E|W|^2\right)$
- Can show this converges to a fixed point: $\eta = MSE^*\left(\frac{N}{M}\eta + E|W|^2\right)$
- Optimal MMSE for the original vector problem: $\eta_{opt} = \lim_{N\to\infty} \frac{1}{N}\|x_0 - E(x_0|y)\|^2$
- Theorem: In the Large System Limit, the true optimal MMSE satisfies:

$$\eta_{opt} = MSE^*\left(\frac{N}{M}\eta_{opt} + E|W|^2\right)$$

  - Conjectured originally by the replica method in statistical physics [Guo-Verdu 05]
  - Proven rigorously by [Reeves, Pfister 16], [Barbier, Dia, Macris, Krzakala 16]
- Conclusion: If the fixed point is unique, MMSE-AMP is optimal!

Story So Far

- AMP is computationally simple:
  - Multiplication by A and A^T and scalar estimators
- Applies to general class of problem: Any i.i.d. prior
- For large i.i.d. Gaussian matrix A:
  - Can be exactly analyzed via state evolution
  - Gives optimal performance when SE equations have unique fixed point
  - Holds true even in non-convex multi-modal problems
- Up soon: What happens outside the i.i.d. Gaussian matrix A case?

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Belief Propagation and AMP

Problem → AMP-like algorithm → Proof that works (or is optimal)

BP: "Derive" an algorithm

Bolthausen conditioning, Replica, …

- AMP was originally "derived" as an approximation to Belief Propagation
- But, BP proof techniques do not generally apply to AMP problems
- So we use BP to derive algorithms
  - Use other methods to analyze them
- Here, we present BP to derive a generalization of AMP called GAMP

Estimation in High Dimensions

- Belief propagation is for problems in high dimensions
- Consider random vector $x = (x_1, \ldots, x_N)$ with posterior density $p(y|x)$ and
- Want to estimate x from y:
  - ML: $\hat{x} = \arg\max_x p(y|x)$
  - MAP: $\hat{x} = \arg\max_x p(x|y)$
  - Posterior mean / MMSE: $\hat{x} = E(x|y)$
- Curse of Dimensionality: Estimate complexity grows exponentially in N
  - Brute force summation / maximization are not possible at moderate N
  - Need approximate methods or some other structure
- Explain a little more

Belief Propagation: Divide and Conquer

- AMP methods are based on belief propagation (next section)
- Key idea in BP: Many densities have a factorizable structure
- Posterior density $p(x|y)$ on vector $x = (x_1, \dots, x_N)$ can be written as:

$$p(x|y) = \frac{1}{Z(y)} \exp[-H(x,y)], \qquad H(x,y) = \sum_i f_i(x,y)$$

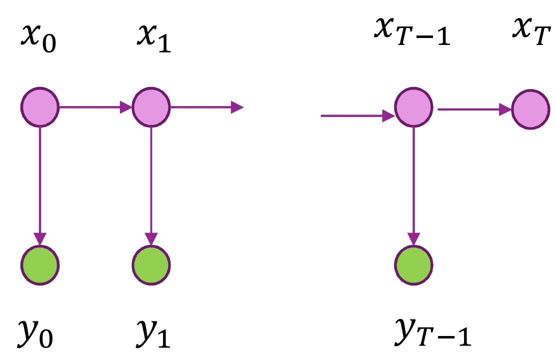
  - $H(x,y)$ is called the energy function
  - Each factor $f_i(x,y)$ assumed to depend only small number of components of x and y
- Belief propagation: Reduces estimation problem on x onto sub-problems of each factor
  - If factors have small numbers of components, estimation is tractable
  - May be approximate…

Ex 1: Estimation in a Hidden Markov Chain

- Markov chain: $x = (x_0, \ldots, x_T)$, $x_t \in R^d$
- Observations $y = (y_0, \ldots, y_{T-1})$
- Problem: Estimate sequence x from y
  - Applications: Dynamical systems, control, time series, …
- By Markov property:

$$\ln p(x, y) = \sum_{t=0}^{T-1} \ln p(x_{t+1}|x_t) + \sum_{t=0}^{T-1} \ln p(y_t|x_t)$$

- Energy function $H(x, y) = -\ln p(x, y)$ factorizes:
  - Total dimension of $x = d(T+1)$
  - T factors of dimension $2d$ and T factors of dimension d



Ex 2: TV Image Denoising

- Image denoising: Estimate image $x = (x_{ij})$ from noisy version $y = x + w$
- TV denoising: Minimize prediction + gradients

$$\hat{x} = \arg\min_x H(x,y), \qquad H(x,y) = \frac{1}{2}\|y-x\|^2 + \lambda\|G_1 x\|_1 + \lambda\|G_2 x\|_1$$

- Cost function is factorizable:

$$H(x,y) = \frac{1}{2}\sum_{ij} |y_{ij} - x_{ij}|^2 + \lambda \sum_{ij} |x_{i+1,j} - x_{ij}|^2 + \lambda \sum_{ij} |x_{i,j+1} - x_{ij}|^2$$

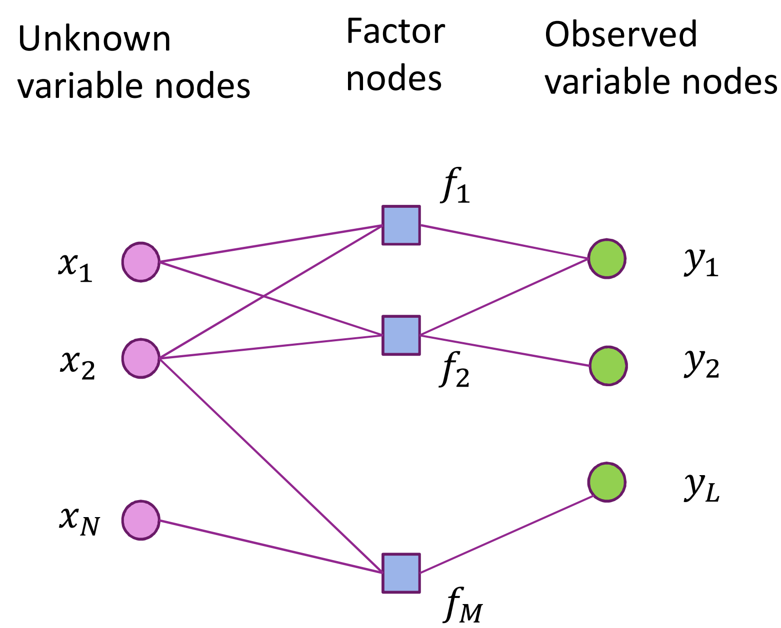
  - Unknown x is typically high-dimensional (e.g. 512 x 512 = 2^{18} components)
  - But, each factor involves only 1 or 2 pixels
  - Differences between neighboring pixels
  - Differences with true pixel value x_{ij} and observed y_{ij}

Factor Graphs

- Assume $x \in R^N, y \in R^L$
- Assume energy function factorizes:

$$H(x, y) = \sum_{i=1}^{M} f_i(x_{a(i)}, y_{b(i)})$$

  - Factors $f_i(\cdot), i = 1, \ldots, M$
  - $a(i) \subset \{1, \ldots, N\}, b(i) \subset \{1, \ldots, L\}$ components in factor i



- Factor graph:
  - Graphical representation of dependencies
  - Undirected, bipartite graph
  - Edge (i, j) in graph $\Leftrightarrow j \in a(i)$, (i, ℓ) in graph $\Leftrightarrow \ell \in b(i)$
  - Let $d(j)$ = neighbors of x_j
- Note: Add example on next slide

Max-Sum and Sum-Product BP

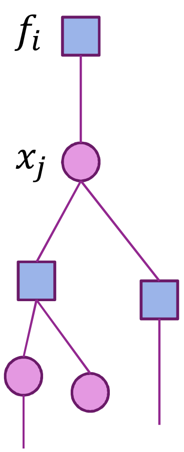
- Consider factorizable posterior density:

$$p(x|y) = \frac{1}{Z(y)} \exp[-H(x)], \qquad H(x) = \sum_{i=1}^{M} f_i(x_{a(i)}), \qquad \psi_i\left(x_{a(i)}\right) := e^{-f_i\left(x_{a(i)}\right)}$$

  - Suppressed dependence on observed variables y
- Two variants of BP, depending on problem
- Sum-product: Estimates posterior marginals $p(x_j|y)$
  - Can compute posterior mean / MMSE estimate $E(x|y)$ from the marginals
- Max-sum: MAP estimation $\hat{x} = \arg\max_x p(x|y) = \arg\min_x H(x)$
  - Can also be viewed as function minimization with no probabilistic interpretation
- Will focus on sum-product

Acyclic Factor Graphs

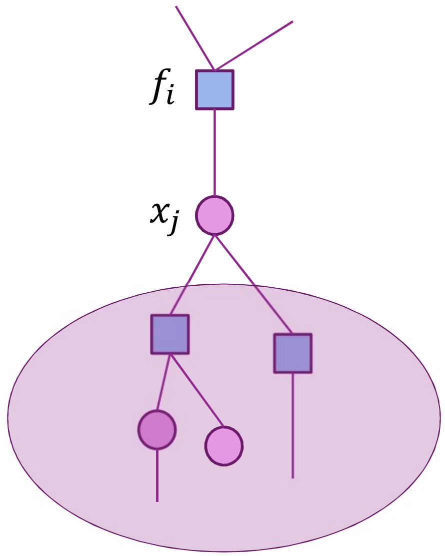
- Suppose factor graph is acyclic (i.e. no loops) and connected
- Acyclic, connected graph can be written as a tree.
  - Can select any node as root.
- Belief propagation on a tree: Max-sum and sum-product are exact!
- Based on message passing
  - Messages from variables to factor nodes
  - Messages from factor to variable nodes
  - Each message is a partial MAP or density estimate
- Will illustrate for sum-product



Sum-Product Messages on the Factor Graph

- Variable x_j to factor f_i:

$$b_{i\leftarrow j}(x_j) \propto \prod_{k \in T_{i\leftarrow j}} \psi_k(x_{a(k)})$$

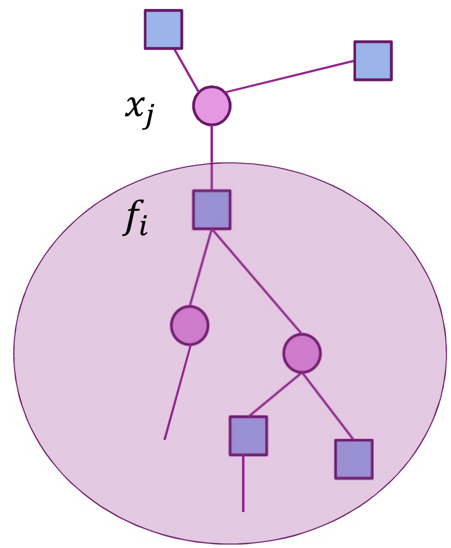


$T_{i\leftarrow j}$ Subtree:

Nodes connected to x_j w/o going via f_i

- Factor f_i to variable x_j:

$$b_{i\leftarrow j}(x_j) \propto \prod_{k \in T_{i\rightarrow j}} \psi_k(x_{a(k)})$$



$T_{i\rightarrow j}$ Subtree:

Nodes connected to f_i w/o going via x_j

Recursive Formula for Sum-Product

- Easy to verify properties on a tree:
  - For any leaf node: $b_{i\leftarrow j}(x_j) = 1$ and $b_{i\rightarrow j}(x_j) = \psi_i(x_j)$
  - For all messages from variable nodes:

$$b_{i\leftarrow j}(x_j) \propto \prod_{k\in d(j)\backslash \mathrm{i}} b_{k\rightarrow j}(x_j)$$

  - For all messages from factor nodes:

$$b_{i\rightarrow j}(x_j) \propto \sum_{x_k, k\in a(i)\backslash \mathrm{j}} \psi_i(x_{a(i)}) \prod_{k\in a(i)\backslash \mathrm{j}} b_{i\leftarrow k}(x_k)$$

  - Final posterior marginal can be computed from:

$$b(x_j) \propto \prod_{k\in d(j)} b_{k\rightarrow j}(x_j)$$

BP on a Tree

- Recursive equations enables simple algorithm for exact inference
- Select any root node and form a tree
  - For all leaf nodes, set messages: $b_{i\leftarrow j}(x_j) = 1$ and $b_{i\rightarrow j}(x_j) = \psi_i(x_j)$
- Compute messages recursively from leaf nodes to root:

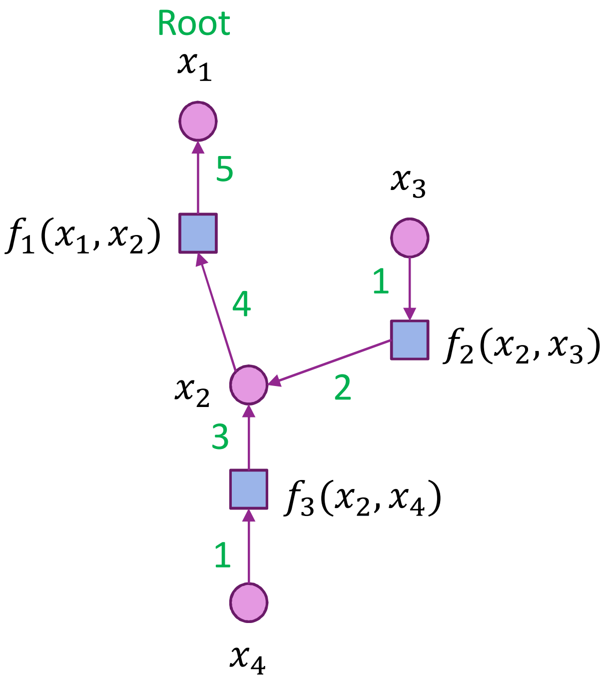
$$b_{i\rightarrow j}(x_j) \propto \sum_{x_k, k\in a(i)\setminus j} \psi_i(x_{a(i)}) \prod_{k\in a(i)\setminus j} b_{i\leftarrow k}(x_k), \qquad b_{i\leftarrow j}(x_j) \propto \prod_{k\in d(j)\setminus i} b_{k\rightarrow j}(x_j)$$

- Then, compute messages from root back to leaves
- Compute final estimates

$$b(x_j) \propto \prod_{k\in d(j)} b_{k\rightarrow j}(x_j)$$

Example: Messages to Root Node

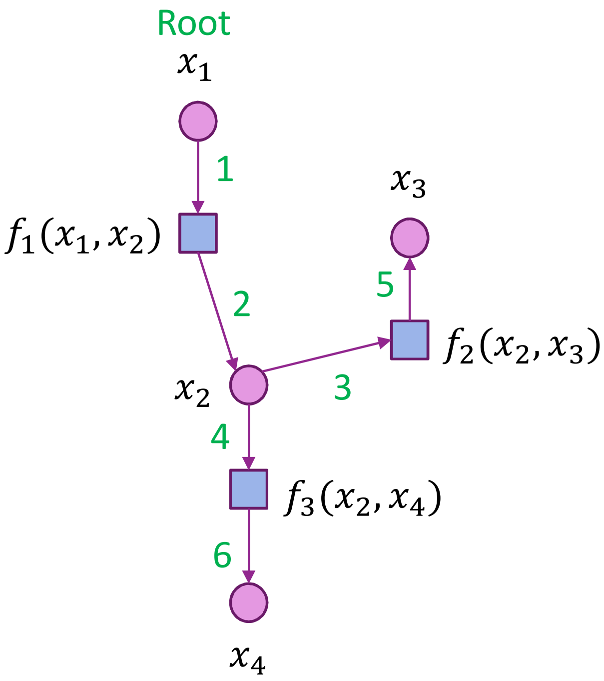
- Pick root node x_1 (you can pick any node)
- Recursively compute message to root:
  1. Initialize $\mu_{3\leftarrow 4}(x_4) = 0, \mu_{2\leftarrow 3}(x_3) = 0$
  2. Compute $\mu_{2\rightarrow 2}(x_2)$ from $\mu_{2\leftarrow 3}(x_3)$ and $f_2(x_2, x_3)$
  3. Compute $\mu_{3\rightarrow 2}(x_2)$ from $\mu_{3\leftarrow 4}(x_4)$ and $f_3(x_2, x_4)$
  4. Compute $\mu_{1\leftarrow 2}(x_2) = \mu_{2\rightarrow 2}(x_2)+ \mu_{3\rightarrow 2}(x_2)$
  5. Compute $\mu_{1\rightarrow 1}(x_1)$ from $\mu_{1\leftarrow 2}(x_2)$ and $f_1(x_1, x_2)$



Example: Messages to Leaf Nodes

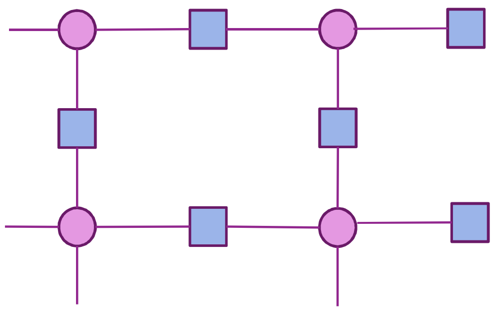
- Recursively compute messages to leaf nodes:
  1. Initialize $\mu_{1\leftarrow 1}(x_1) = 0$,
  2. Compute $\mu_{1\to 2}(x_2)$ from $\mu_{1\leftarrow 1}(x_1)$ and $f_1(x_1, x_2)$
  3. Compute $\mu_{2\leftarrow 2}(x_2) = \mu_{1\to 2}(x_2) + \mu_{3\to 2}(x_2)$
  4. Compute $\mu_{3\leftarrow 2}(x_2) = \mu_{1\to 2}(x_2) + \mu_{2\to 2}(x_2)$
  5. Compute $\mu_{2\to 3}(x_3)$ from $\mu_{2\leftarrow 2}(x_2)$ and $f_2(x_2, x_3)$
  6. Compute $\mu_{3\to 4}(x_4)$ from $\mu_{3\leftarrow 2}(x_2)$ and $f_3(x_2, x_4)$

- Compute estimates:
  - $\hat{x}_1 = \arg\min_{x_1} \mu_{1\to 1}(x_1)$
  - $\hat{x}_2 = \arg\min \mu_{1\to 2}(x_2) + \mu_{2\to 2}(x_2) + \mu_{3\to 2}(x_2)$
  - $\hat{x}_3 = \arg\min \mu_{2\to 3}(x_3)$
  - $\hat{x}_4 = \arg\min \mu_{3\to 4}(x_4)$



Graphs with Loops

- Problem: In many problems, graph has loops
  - Ex: For TV denoising, graph is a lattice structure
- Loopy belief propagation: Approximate solution
  - Apply same recursions as BP with trees for messages
- Typically iterations:
  1. Initialize $b_{i\leftarrow j}(x_j) = 1$
  2. Factor node update:
  $$b_{i\rightarrow j}(x_j) \propto \sum_{x_k, k\in a(i)\backslash \mathrm{j}} \psi_i(x_{a(i)}) \prod_{k\in a(i)\backslash \mathrm{j}} b_{i\leftarrow k}(x_k)$$
  3. Variable node update:
  $$b_{i\leftarrow j}(x_j) \propto \prod_{k\in d(j)\backslash \mathrm{i}} b_{k\rightarrow j}(x_j)$$
  4. Repeat Step 2 and 3 until convergence



Loopy Belief Propagation Issues

- Potential shortcomings:
  - Loopy BP may diverge
  - When it converges, no guarantee that estimate is correct
- Considerable work to find convergence guarantees / approximation bounds
  - Locally tree like conditions
  - Dorbrushin condition (weak coupling)
- AMP will be derived from loopy BP
  - But, we prove its convergence via state evolution

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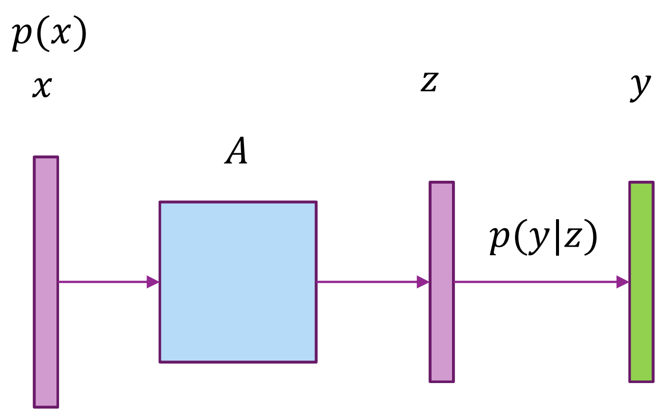
- Convergence, Fixed Points and Stability
- Extensions: Vector AMP
- Thoughts on What is Next

GLM Estimation

- Will look at AMP in a more general setting
- Bayesian Generalized linear model (GLM):
  - IID prior $p(x) = \prod_j p(x_j)$
  - Linear transform: $z = Ax$
  - Componentwise likelihood: $p(y|z) = \prod_i p(y_i|z_i)$
- Problem: Estimate x and z from A and y
- Linear inverse problem is a special case:

$$y = z + w, \qquad w \sim N(0, \sigma^2 I)$$

- But, GLM can incorporate:
  - Nonlinearities in outputs
  - Outputs can be discrete
  - Non-Gaussian noise

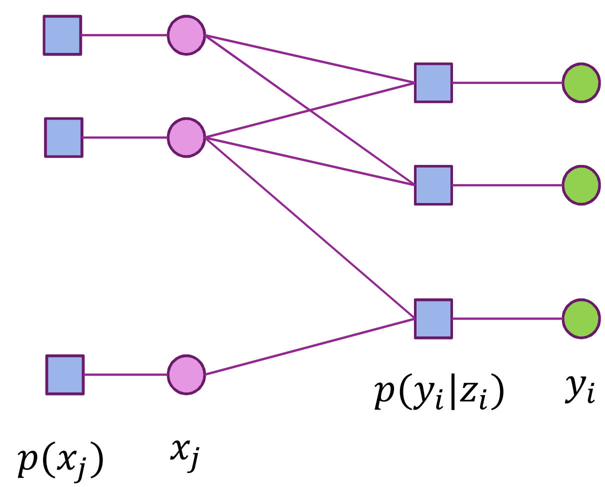


Factor Graph for a GLM

- Posterior density factors as:

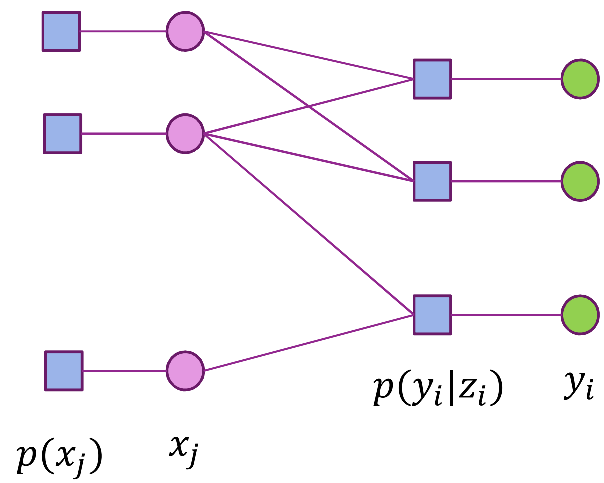
$$p(x|y) = \frac{1}{Z(y)} \prod_j p(x_j) \prod_i p(y_i|z_i), \qquad z_i = A_i^T x = \sum_j A_{ij} x_j$$

- Problem applying BP directly:
  - Factor graph has loops
  - Graph is dense if A is dense
  - Messages must be over variables x_j
- Can we still get approximate inference using BP?
  - Will it converge?
  - Can it be optimal?



Sum-Product BP for GLM

- Consider sum-product (Loopy) BP for the GLM problem
- With slight rearrangement, updates can be written in two stages



- Output node updates:

$$b_{i\to j}(x_j) \propto E\{p(y_i|z_i)|x_j,\ x_k \sim b_{i\leftarrow k}(x_k)\}, \qquad z_i = \sum_j A_{ij} x_j$$

  - Message from factors $p(y_i|z_i)$ to variables x_j

- Input node updates:

$$b_{i\leftarrow j}(x_j) \propto p(x_j) \prod_i b_{i\to j}(x_j)$$

  - Message from variables x_j to factors $p(y_i|z_i)$

GAMP Approximations

- Assume that each A_{ij} is relatively small

$$\frac{|A_{ij}|^2}{\sum_k |A_{ik}|^2} = O\left(\frac{1}{N}\right), \qquad \frac{|A_{ij}|^2}{\sum_k |A_{kj}|^2} = O\left(\frac{1}{N}\right)$$

  - Applies to dense matrices where all components are roughly same value
- Under this assumption:
  - Apply a Central Limit Theorem approximation in the output update
  - A second order approximation of the messages in the input update
- The approximation is heuristic
  - No rigorous bound for discrepancy between full BP and AMP
  - Full BP is approximate anyway (since graph has loops)
- Used as motivation for the algorithm
- Can analyze rigorously via state evolution

Output Node Approximation

- Output update

$$b_{i\to j}(x_j) \propto E\{p(y_i|z_i)\big|x_j,\ x_k \sim b_{i\leftarrow k}(x_k)\}, \qquad z_i = \sum_j A_{ij}x_j$$

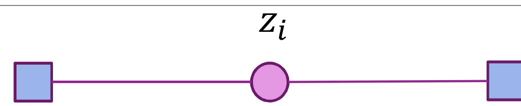
- Define mean and variance of each incoming msg: $\hat{x}_{i\leftarrow j} = E\left(x_j \middle| b_{i\leftarrow j}\right),\ \tau^x_{i\leftarrow j} := var\left(x_j \middle| b_{i\leftarrow j}\right)$
- Apply Central Limit Theorem: Since incoming messages are independent:

$$b_{i\to j}(x_j) \approx \frac{1}{Z} E\left\{p(y_i|z_i)\middle| z_i \sim N(p_{i\to j}, \tau^p_{i\to j})\right\}$$

- Mean and variance on z_i given by:
  - $p_{i\to j} := p_i + A_{ij}\left(x_j - \hat{x}_{i\leftarrow j}\right),\ p_i := \sum_k A_{ik}\,\hat{x}_{i\leftarrow k},$
  - $\tau^p_{i\to j} = \sum_{k\neq j} A^2_{ik}\tau^p_{i\leftarrow k}$

Scalar Output Channel

Gaussian Prior $z_i \sim N(z_i|p_i, \tau_i^p)$



Measurement $y_i \sim P(y_i|z_i)$

- Scalar output estimation problem: Estimate z_i, Gaussian prior on z_i, measurement y_i
- Posterior density is:

$$b_i^z\left(z_i \middle| p_i, \tau_i^p\right) := \frac{1}{Z(p_i, \tau_i^p, y_i)} p(y_i|z_i) N(z_i|p_i, \tau_i^p)$$

- Log likelihood of y_i is $G_i\left(p_i, \tau_i^p, y_i\right) := \ln E\left\{p(y_i|z_i) \middle| z_i \sim N\left(p_i, \tau_i^p\right)\right\} = \ln Z_i(p_i, \tau_i^p, y_i)$
- Using properties of exponential families, can show:

$$G_i'\left(p_i, \tau_i^p\right) = E\left[z_i \middle| p_i, \tau_i^p\right], \qquad G_i''\left(p_i, \tau_i^p\right) = -\frac{1}{\tau_i^p}\left[1 - \frac{var\left[z_i \middle| p_i, \tau_i^p\right]}{\tau_i^p}\right]$$

  - Derivatives are with respect to p_i

Input Node Approximation

- Consider logarithmic message: $\mu_{i\to j}(x_j) = -\ln b_{i\to j}(x_j)$
- By output update:

$$\mu_{i\to j}(x_j) = -\ln E\left\{p(y_i|z_i)\middle|z_i \sim N\left(p_{i\to j}, \tau^p_{i\to j}\right)\right\} \approx -G_i\left(p_i + A_{ij}(x_j - \hat{x}_{i\leftarrow j}), \tau^p_{i\to j}, y_i\right)$$

- If A_{ij} is small:

$$\mu_{i\to j}(x_j) \approx -G_i\left(p_i, \tau^p_{i\to j}\right) - G_i'\left(p_i, \tau^p_{i\to j}\right)A_{ij}(x_j - \hat{x}_{i\leftarrow j}) - \frac{1}{2}G_i''\left(p_{i\to j}, \tau^p_{i\to j}\right)A_{ij}^2(x_j - \hat{x}_{i\leftarrow j})^2$$

- Input node update:

$$b_{i\leftarrow j}(x_j) = \frac{1}{Z}p(x_j)\exp\left[-\sum_{k\neq i}\mu_{i\to k}(x_j)\right] \approx \frac{1}{Z}p(x_j)\exp\left[-\frac{(x_j - r_{i\leftarrow j})^2}{2\tau^r_{i\leftarrow j}}\right]$$

Scalar Input Channel

- Scalar input estimation problem: Estimate x_j with prior on $p(x_j)$ and Gaussian measurement r_j
- Posterior density is:

$$b_j^x\left(x_j \middle| r_j, \tau_j^r\right) := \frac{1}{Z\left(r_j, \tau_j^r\right)} p(x_j) N(r_j | x_j, \tau_j^r)$$

- Message to output nodes are: $b_{i \leftarrow j}\left(x_j\right) = b_j^x\left(x_j \middle| r_{i \leftarrow j}, \tau_{i \leftarrow j}^r\right)$
- For the output node update, we need to compute mean and variance under this density:

$$\hat{x}_{i \leftarrow j} = E\left(x_j \middle| r_{i \leftarrow j}, \tau_{i \leftarrow j}^r\right), \qquad \tau_{i \leftarrow j}^x \coloneqq var\left(x_j \middle| r_{i \leftarrow j}, \tau_{i \leftarrow j}^r\right)$$

Sum-Product GAMP Algorithm

- Combining terms with some more algebra results in simple algorithm

GAMP (Generalized AMP) [Rangan 10]

- Initialization: $\hat{x}_j = E(x_j),\ \tau_j^x = var(x_j)$ from prior $p(x_j)$
- Repeat until convergence:
  - Forward linear transform: $p_i = \sum_j A_{ij}\hat{x}_j - \tau_i^p s_i,\ \ \tau_i^p = \sum_j |A_{ij}|^2 \tau_j^x$
  - Output estimation: $\hat{z}_i = E\left(z_i \middle| p_i, \tau_i^p\right),\ \ \tau_i^z = var\left(z_i \middle| p_i, \tau_i^p\right)$
  - Reverse nonlinear transform : $s_i = \frac{1}{\tau_i^p}[\hat{z}_i - p_i],\ \ \tau_i^s = \frac{1}{\tau_i^p}\left[1 - \frac{\tau_i^z}{\tau_i^p}\right]$
  - Reverse linear transform: $r_j = \hat{x}_j - \tau_j^r \sum_i A_{ij} s_i\ ,\ \ \tau_j^r = \left(\sum_i |A_{ij}|^2 \tau_j^s\right)^{-1}$
  - Input node estimation: $\hat{x}_j = E\left(x_j \middle| r_j, \tau_j^r\right),\ \ \tau_j^x = var\left(x_j \middle| r_j, \tau_j^r\right)$

Scalar Variance GAMP

- Make approximation that all variances are constant: e.g. $\tau_j^x \approx \tau^x$
- Resulting algorithm:
  - Forward linear transform: $p = A\hat{x} - \tau^p s, \quad \tau^p = \frac{1}{M}\|A\|_F^2 \tau^x$
  - Output estimation: $\hat{z} = g_{out}(p, \tau_p), \quad \tau^z = \tau^p \langle g_{out}'(p, \tau_p) \rangle$
  - Reverse nonlinear transform : $s = \frac{1}{\tau^p}[\hat{z} - p], \quad \tau^s = \frac{1}{\tau^p}\left[1 - \frac{\tau^z}{\tau^p}\right]$
  - Reverse linear transform: $r = \hat{x} - \tau^r A^T s, \quad \tau^r = N\left(\|A\|_F^2 \tau^s\right)^{-1}$
  - Input node estimation: $\hat{x} = g_{in}(r, \tau_r), \quad \tau^r = \tau^r \langle g_{in}'(r, \tau_r) \rangle$

From GAMP to AMP

- Special case of an AWGN output: $y = z + w, \quad w \sim N(0, \tau_w I)$
- Output estimator:
  - $g_{out}(p, \tau^p) = \frac{1}{\tau_p + \tau_w}(\tau_w p + \tau_p y), \; g'_{out}(p, \tau^p) = \frac{\tau_p \tau_w}{\tau_p + \tau_w}$
- Then, we obtain AMP with specific choice of thresholding
  - Forward linear transform: $p = A\hat{x} - \tau^p s, \quad \tau^p = \frac{1}{M}\|A\|_F^2 \tau^x$
  - Residual: $s = \frac{1}{\tau^p + \tau^w}(y - p), \quad \tau^s = \frac{1}{\tau^p + \tau^w}$
  - Reverse linear transform: $r = \hat{x} - \frac{N}{\|A\|_F^2} A^T (y - p), \quad \tau^r = \frac{N}{\|A\|_F^2}(\tau^p + \tau^w)$
  - Input node estimation: $\hat{x} = g_{in}(r, \tau_r), \quad \tau^r = \tau^r \langle g'_{in}(r, \tau_r) \rangle$

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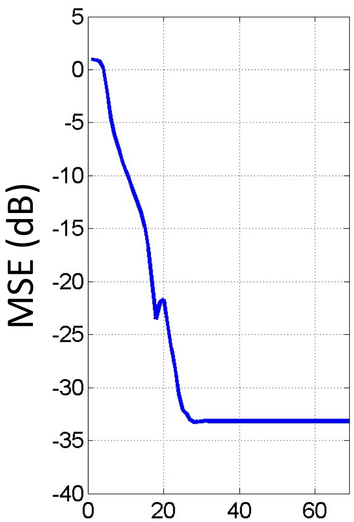
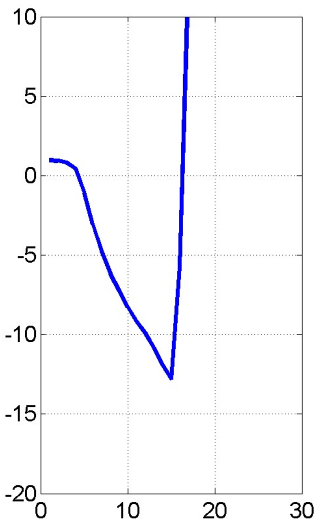
Problems with AMP for Non-IID A

A = iid, N(0,1)



Converges rapidly

A = iid N(0.5,1)

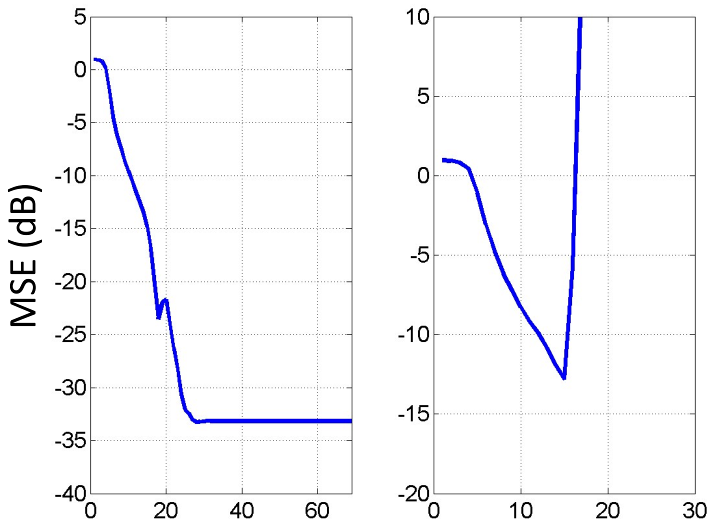


Diverges

- *Evidently, this promise comes with the caveat that message-passing algorithms are specifically designed to solve sparse-recovery problems for Gaussian matrices…”,* Felix Herman, Nuit Blanche blog, 2012
- AMP can diverge for non-iid A
- Even non-pathological matrices
- See [FZK14]

Questions for This Section

A = iid, N(0,1) **A** = iid N(0.5,1)



Converges rapidly

Diverges

- ❑When exactly does AMP converge?
- ❑What does it converge to, if it does?
- ❑Can convergence be improved?

GAMP on a Gaussian Problem

- Consider simple Gaussian problem:
  - $x \sim N(0, \tau_x I),\ y = Ax + w,\ w \sim N(0, \tau_w I)$
- Question: When does AMP/GAMP converge for this problem?
  - Convergence of second-order / variance terms
  - Convergence of first-order / mean terms
- GAMP is not the best solution for Gaussian problem
  - MMSE solution has explicit solution: $\hat{x} = \tau_x(\tau_x A^T A + \tau_w I)^{-1} A^T y$
- Look at Gaussian problem since:
  - Can derive exact conditions for convergence
  - Convergence conditions are easy to interpret

Rangan, Schniter, Fletcher. "On the convergence of approximate message passing with arbitrary matrices." *Proc IEEE ISIT 2014*

Variance Convergence

- AWGN vector-valued variance updates:

$$\tau_p^t = S\tau_x^t, \qquad \tau_s^t = \frac{1}{\tau_p^t + \tau_w},$$

$$\tau_r^t = \frac{1}{S^* \tau_s^t}, \qquad \tau_x^{t+1} = \frac{\tau_r^t \tau_0}{\tau_r^t + \tau_0}$$

  - $S = |A|^2$ = componentwise magnitude squared

- Theorem: For any τ_w and τ_0, the AWGN variance updates converge to unique fixed points

- Subsequent results will consider algorithm with fixed variance vectors.

Proof of the Variance Convergence

- Define vector valued functions:

$$g_s: \tau_x^t \mapsto \tau_s^t, \qquad g_x: \tau_s^t \mapsto \tau_x^{t+1}, \qquad g = g_x \circ g_s$$

- Verify g satisfies:
  - Monotonically increasing
  - $g(\alpha \tau_s) \leq \alpha g(\tau_s)$ for $\alpha \geq 1$.

- Convergence now follows from R. D. Yates, "A framework for uplink power control in cellular radio systems", 1995
  - Used for convergence of power control loops

Convergence of the Means
Uniform Variance Update

- Consider constant case:
  - Constant variances: $\tau_{0j} = \tau_0,\ \tau_{wi} = \tau_w$.
  - Uniform variance updates in GAMP

- Theorem: The means of the AWGN GAMP will converge for all τ_0 and τ_w if and only if

$$\sigma_{max}^2(A) < \frac{2(m+n)}{mn}\|A\|_F^2$$

  - $\sigma_{max}(A)$: maximum singular value
  - $\|A\|_F^2$ = Frobenius norm = sum of singular values

Some Matrices Work…

$$\sigma_{max}^2(A) < \frac{2(m+n)}{mn} \|A\|_F^2$$

- Convergence depends on bounded spread of singular values.

- Examples of convergent matrices:
  - Random iid: Converges due to Marcenko-Pastur
  - Subsampled unitary: $\sigma_{max}^2(A)$=1, $\|A\|_F^2 = \min(m,n)$
  - Total variation operator: $(Ax)_i = x_i - x_{i-1}$
  - Walk summable matrices: Generalizes result by Maliutov, Johnson and Willsky (2006)

But, Many Matrices Diverge

$$\sigma_{max}^2(A) < \frac{2(m+n)}{mn} \|A\|_F^2$$

- Examples of matrices that do not converge:
  - Low rank: If A has r equal singular values and other are zero:
  $$2r(m+n) > mn \Rightarrow r > \min(m,n)/2$$
  - $A \in R^{m\times m}$ is a linear filter: $Ax = h * x$ for some filter h
  $$\sup_\theta \left|H\left(e^{i\theta}\right)\right| < \frac{1}{2}\ \frac{1}{2\pi}\int \left|H\left(e^{i\theta}\right)\right|^2 d\theta$$
  - Some matrices with large non-zero means: $A = A_0 + \mu 1^T$

Proof of Convergence

- With constant variances system is linear:

$$\begin{bmatrix} s^t \\ x^{t+1} \end{bmatrix} = G \begin{bmatrix} s^{t-1} \\ x^t \end{bmatrix} + b$$

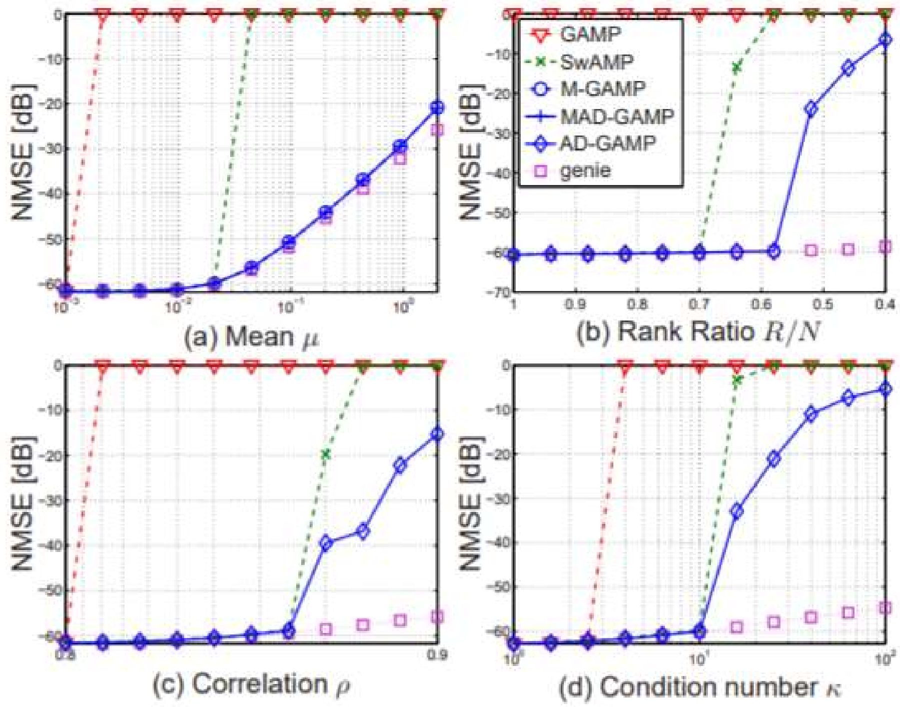
  - $G = \begin{bmatrix} I & 0 \\ D(\tau_x)A^* & D(\tau_x \tau_r^{-1}) \end{bmatrix} \begin{bmatrix} D(\tau_p \tau_s) & -D(\tau_s)A \\ 0 & I \end{bmatrix}$
  - $D(\tau) = diag(\tau)$

- System is stable if and only if $\lambda_{max}(G) < 1$
- Eigenvalue condition related to singular values of

$$F = D\left(\tau_s^{1/2}\right) AD\left(\tau_x^{1/2}\right)$$

Improving Stability

- Many methods
  - Coordinate-wise descent [MKTZ14,CKZ14]
  - Damping [VSR+14, JBD09]
  - Double loop / ADMM [RSF17]
- Slow rate with improved robustness
- But:
  - May still fail
  - Often needs tuning



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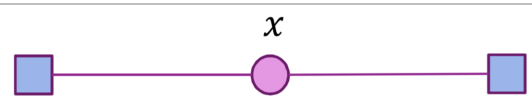
Story So Far

- Benefits of AMP: For large Gaussian i.i.d. A
  - Fast convergence
  - Can be analyzed rigorously via state evolution
  - Testable conditions for optimality
- But, outside Gaussian i.i.d. A:
  - Can diverge.
  - Stability techniques are only partially successful
  - Loses key properties
- Is there a better way?

A Vector Valued Factor Graph

Prior $p(x)$



Measurement $y = Ax + w,\ w \sim N(0, \gamma_w^{-1} I)$

- Consider simpler factor graph for linear inverse problem:
  - Single vector variable node for x
  - One factor for prior $\psi_1(x) \coloneqq p(x)$ (separable)
  - One factor for likelihood $\psi_2(x) \coloneqq p(y|x)$ (Gaussian)
- Posterior density factors as:

$$p(x|y) = \frac{1}{Z(y)} \psi_1(x) \psi_2(x)$$

- Insight due to [Cakmak, Winther, Fleury, 14, 15]

Variational Inference

- Write posterior as:

$$p(x|y) = \frac{1}{Z(y)}\psi_1(x)\psi_2(x), \qquad \psi_1(x) = p(x), \qquad \psi_2(x) = p(y|x)$$

- Variational inference:

$$\hat{b} = \arg\min_b D(b(\cdot)||p(\cdot\,|y)) = \arg\min_b [D(b\|\psi_1) + D(b\|\psi_2) + H(b)]$$

- Apply variable splitting:

$$\hat{b}_1, \hat{b}_2 = \arg\min_{b_1,b_2}\max_q J(b_1,b_2,q)\,, \qquad J(b_1,b_2,q) = D(b_1\|\psi_2) + D(b_2\|\psi_1) + H(q)$$

  - Subject to constraints $b_1 = b_2 = q$

- Problem is intractable.
  - Must optimize over N dimensional densities

EC Inference

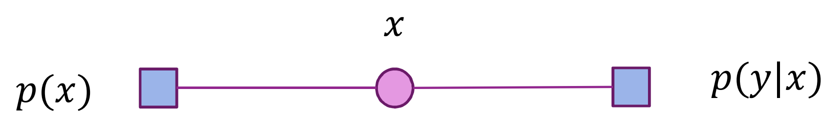
- Desired optimization is too hard:

$$\hat{b}_1, \hat{b}_2 = \arg\min_{b_1,b_2} \max_q J(b_1, b_2, q)\,, \qquad J(b_1, b_2, q) = D(\psi_1 \| b) + D(\psi_2 \| b) + H(b)$$

  - Subject to constraints $b_1 = b_2 = q$
- Expectation consistent inference: Replace constraints by moment matching conditions:
  - $E(x|b_1) = E(x|b_2) = E(x|q)$
  - $E(\|x\|^2|b_1) = E(\|x\|^2|b_2) = E(\|x\|^2|q)$
  - Proposed by Opper-Winther 04, 05
- At EC stationary points:
  - $b_i(x) \propto \psi_i(x) N\left(x \middle| r_i, \gamma_i^{-1} I\right)$, $\quad q(x) = N(x|\hat{x}, \eta^{-1} I)$
  - $E(x|b_1) = E(x|b_2) = E(x|q) = \hat{x}$
  - $E(\|x\|^2|b_1) = E(\|x\|^2|b_2) = E(\|x\|^2|q) = \frac{N}{\eta}$

Vector AMP

- Use Expectation Propagation to find stationary points
- Input Denoising
  - $\hat{x}_1 = g_1(r_1, \gamma_1)$
  - $\eta_1 = \gamma_1/\alpha_1\,,\ \alpha_1 = \langle g_1'(r_1, \gamma_1)\rangle$
  - $\gamma_2 = \eta_1 - \gamma_1,\ r_2 = (\eta_1 \hat{x}_1 - \gamma_1 r_1)/\gamma_2$



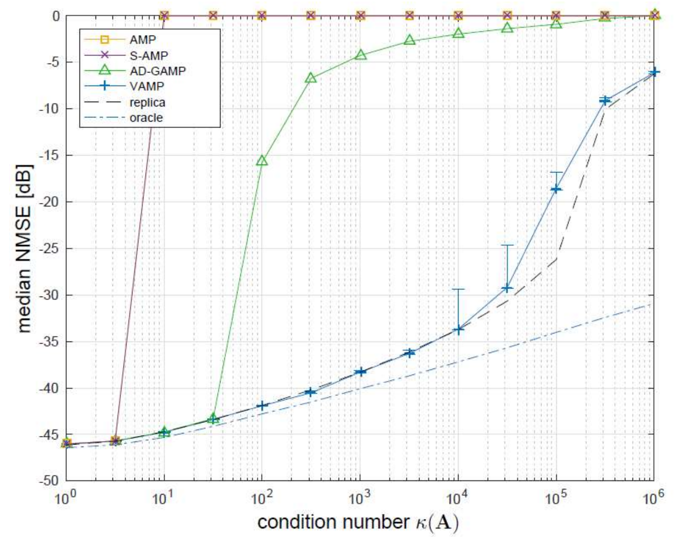
- Denoisers:
  - $g_1(r_1, \gamma_1) = E\left(x \middle| r_1 = x + N\left(0, \gamma_1^{-1}\right),\ x \sim p(x)\right)$
  - $g_2(r_2, \gamma_2) = E\left(x \middle| r_2 = Ax + w,\ x \sim N\left(0, \gamma_2^{-1} I\right)\right)$

- Output Denoising
  - $\hat{x}_2 = g_2(r_2, \gamma_2)$
  - $\eta_2 = \gamma_2/\alpha_2\,,\ \alpha_2 = \langle g_2'(r_2, \gamma_2)\rangle$
  - $\gamma_1 = \eta_2 - \gamma_2,\ r_1 = (\eta_2 \hat{x}_2 - \gamma_2 r_2)/\gamma_1$

Rangan, Schniter, Fletcher, “Vector Approximate Message Passing”, Proc IEEE ISIT 2017

Why Use VAMP?

- Computationally efficient
  - Though harder than AMP.
  - Requires SVD or matrix inverse
- Numerically stable over ill-conditioned matrices
  - Overcomes major problem with AMP
- Performance matches state evolution
  - Achieves replica prediction for optimality
- Extensions: EM, image processing, …



Right-Rotationally Invariant Matrices

- Measurement Model: $y = Ax^0 + w,\ w \sim N(0, \gamma_w^{-1} I)$
- Take SVD: $A = U\mathrm{diag}(s)V^T \in R^{N\times N},\ \ s = (s_1, \ldots, s_N)$
  - WLOG assume A is square (otherwise add zero singular values)
- Left factor U is arbitrary
  - Will assume $U = I$ (Otherwise, look at $U^T y$).
- Right rotationally invariant A :
  - V Haar, uniform on the orthogonal matrices
  - S has limiting distribution
- Includes A Gaussian iid. But, much more general
- New model: $y = \mathrm{diag}(s)V^T x^0 + w,\ w \sim N(0, \gamma_w^{-1} I)$

State Evolution

- Two key error quantities:
  - $p_k = r_{1k} - x^0$: Error on the input to the input denoiser
  - $v_k = r_{2k} - x^0$: Error on the input to the LMMSE denoiser
- Transformed errors: $u_k = V^T p_k, \;\; q_k = V^T v_k$
- Theorem: In large system limit:

$$p_k \to P_k \sim N(0, \tau_k^p), \qquad q_k \to Q_k \sim N(0, \tau_k^q),$$

  - Variances τ_k^p, τ_k^q can be calculated via state evolution
- Shows errors are Gaussian
- Fixed points of SE equations match predictions for optimality from the replica method
  - [Takeda, Uda, Kabishma 06], [Tulino, Caire, Verdu, Shamai 13]
  - Rigorously shown for large subclass in [Barbier, Macris, Maillard, Krzakala 17]

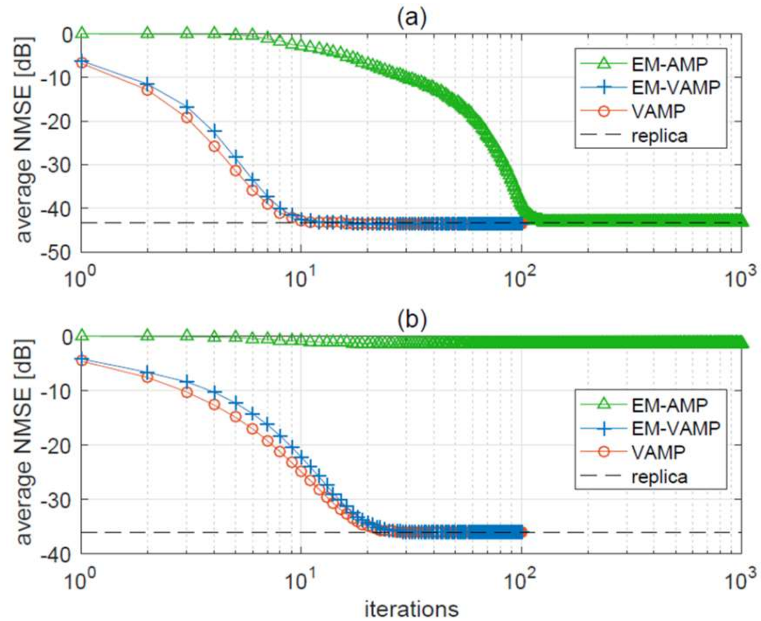
Proof of the SE

- Error recursion
  - $p_k = Vu_k$
  - $v_k = C_1(\alpha_{1k})\left[f_p(p_k, w^p, \gamma_{1k}) - \alpha_{1k}p_k\right],\ \alpha_{1k} = \left\langle f_p'(p_k, w^p, \gamma_{1k})\right\rangle$
  - $q_k = V^T v_k$
  - $u_{k+1} = C_2(\alpha_{2k})\left[f_q(q_k, w^q, \gamma_{2k}) - \alpha_{2k}q_k\right],\ \alpha_{2k} = \left\langle f_q'(q_k, w^q, \gamma_{2k})\right\rangle$
- Similar to Bayati-Montanari recursion but:
  - Gaussian iid A replaced by Haar matrix V
- Can apply Bolthausen conditioning
  - Conditional distribution of Haar matrix V subject to linear constraints $A = VB$

$$V_{|G} = A(A^T A)^{-1}B^T + U_{A^\perp}\tilde{V}U_{B^\perp}$$

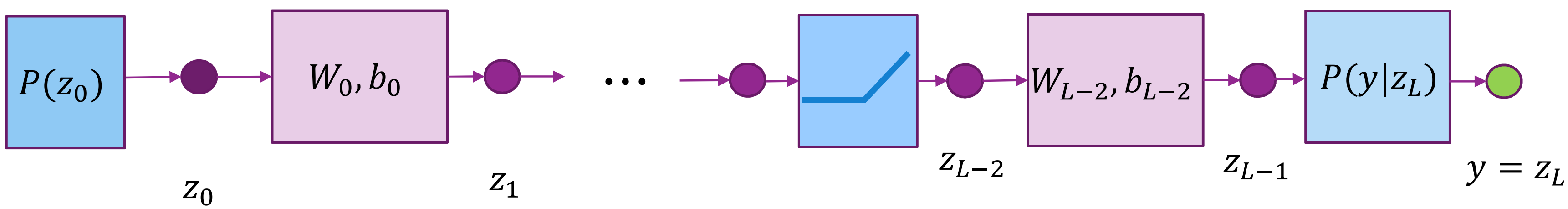
EM VAMP

- Suppose densities have unknown parameters:
  - $x \sim p(x|\theta_1)$
  - $y = Ax + w,\ w \sim N(0, \theta_2^{-1} I)$
- Problem: Estimate x and $\theta = (\theta_1, \theta_2)$
- EM-VAMP:
  - E-Step: Use VAMP to estimate $p\left(x\middle|y, \hat{\theta}\right)$
  - M-Step: $\hat{\theta}^{new} = \arg\max_{\theta} E\left[p(x, y|\theta)|\hat{\theta}\right]$
- Similar ideas in AMP [KrzMSSZ12, VS12]



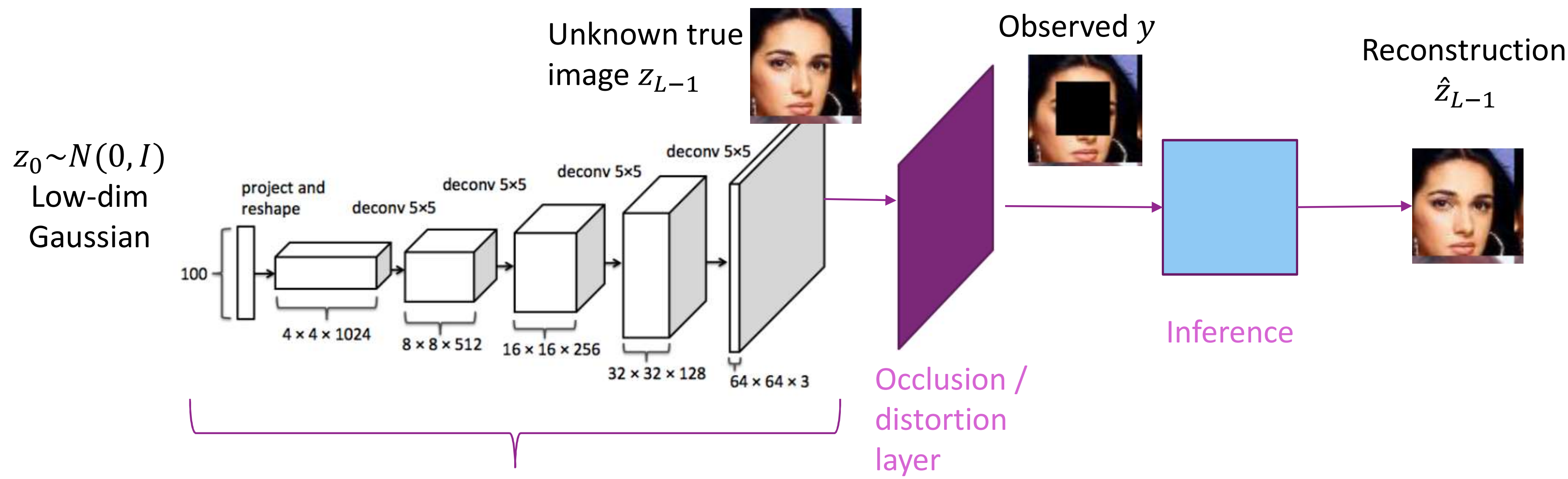
Fletcher, Schniter. "Learning and free energies for vector approximate message passing." *Proc. IEEE ICASSP 2017*

Inference in Deep Networks



- Model:
  - A multi-layer neural network with known weights and biases, activations
  - Distribution on network input $P(z_0)$
  - Network is already trained. Not a learning problem!
- Inference problem: Given observed output $z_L = y$ and network, estimate:
  - Input z_0 and hidden layers $z_1, \ldots, z_{L-1}$
- Network is already trained. Not a learning problem

Motivation: Image Reconstruction



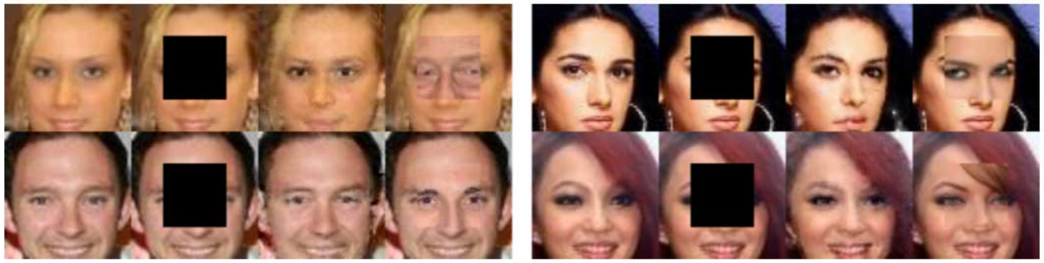
Trained on ensemble of images

Variational autoencoder, Kingma & Welling (2016)

Generative adversarial nets, Goodfellow et al (2014)

Deep convolutional GAN, Radford et al (2015)

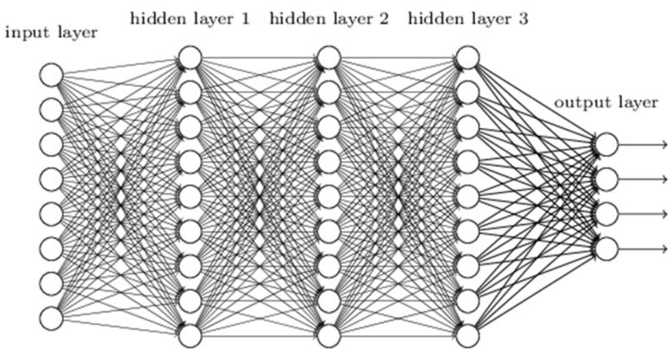
Example Results

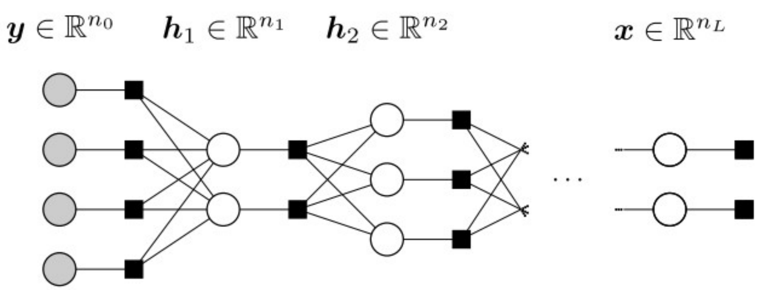


Yeh et al, Semantic Image Inpainting with Perceptual and Contextual Losses, 2016

- Example above:
  - Use DCGAN to train generative model: $x = G(z_0)$ and a discriminator cost $\log(1 - D(G(z_0))$
  - Loss minimized via gradient descent
- Works well in practice, but…
  - Difficult to analyze rigorously
  - Few theoretical guarantees
  - What are the limits on which this works?

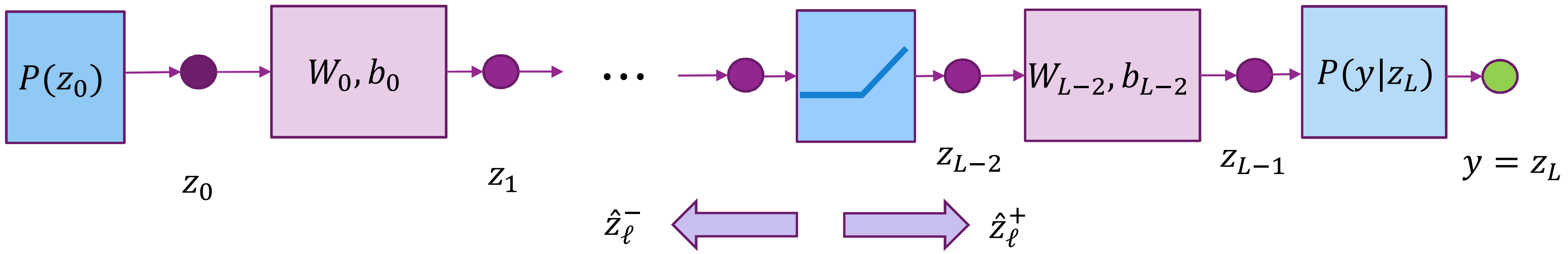
AMP for Multi-Layer Inference





- Use AMP for multi-layer inference
- Proposed by [Manoel, Krzakala, Mezard, Zdeborova, 2017]:
  - Derives simple AMP algorithm
  - Postulates state evolution, free energy, …
  - See also [Gabrié et al, 2016]
- But, limited to Gaussian iid
- Can VAMP do better?

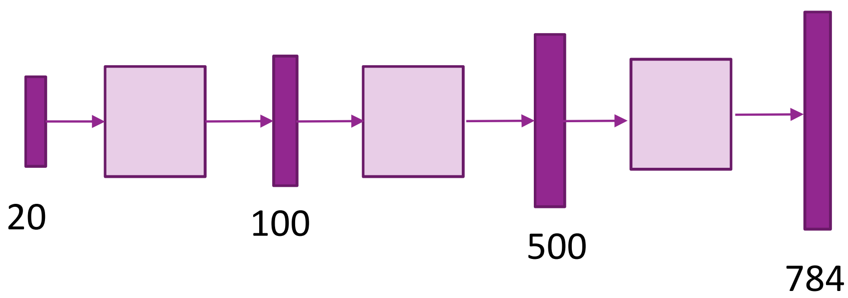
Multi-Layer VAMP



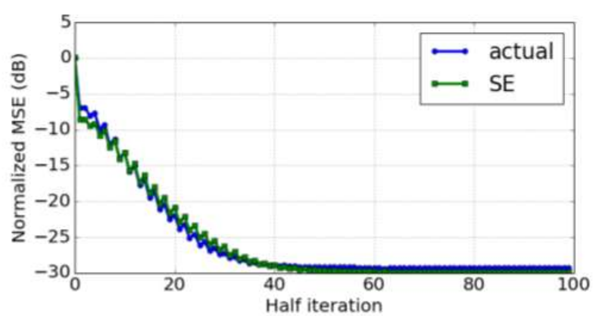
- Multi-layer VAMP: message passing method for multi-layer model
  - Derive with similar EC method as VAMP
  - Extension of [HeWenJin 2017] in GLM model
  - Updates have forward-backward iterations
- Applies to rotationally invariant weight matrices & separable activations
- Can rigorously prove state evolution

Fletcher, Rangan, Schniter. "Inference in deep networks in high dimensions." *Proc IEEE ISIT 2018*

Synthetic Data Example



MSE (dB)

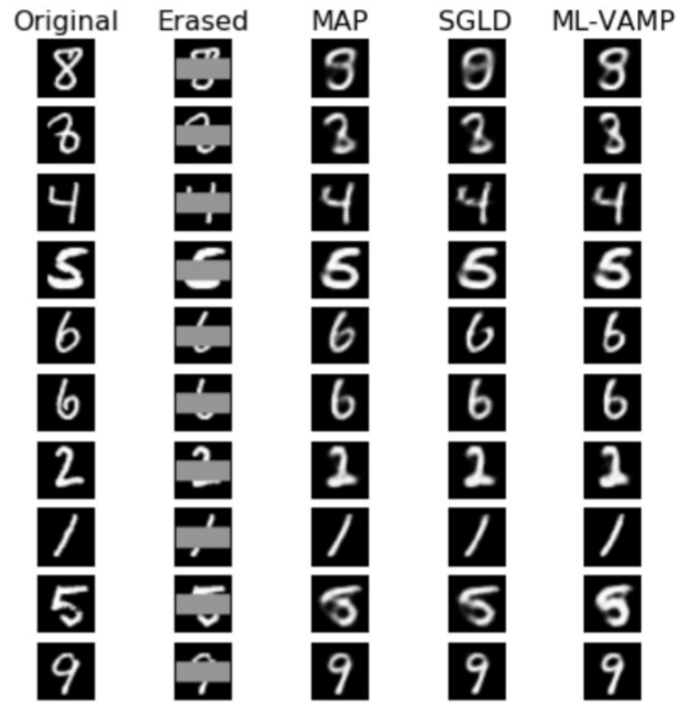


Half Iteration

- Simple network
  - $M = 3$ fully-connected layers
  - ReLU activations $z_{2m+1} = \max(z_{2m}, 0)$
- Random parameters
  - Gaussian iid W_0, W_1. Rotationally invariant W_2
  - Biases selected for sparsity at ReLU output
- Output AWGN at SNR=20 dB
- Good final estimate of posterior variance

Toy MNIST Inpainting

- Train network via VAE
  - Fully connected layers + ReLUs
  - 20 input variables
  - 400 hidden units
  - 784 dim output
- Perform ML-VAMP for inference
  - Need damping for stability
- Faster convergence:
  - MAP with ADAM optimizer: ~400 iterations
  - SGLD: ~20000 iterations
  - ML-VAMP: ~20 iterations



What is Known

Model	Iid Gaussian		Orthogonally Invariant	
	Algorithmic SE	Fundamental limit	Algorithmic SE	Fundamental limit
Linear	[DMM10,BM09]	[GV05,**RP16, BDMK16**]	[CVF14,RSF16]	[TUK06,TCVS13, BMMK17]
GLM	[Ran10,JavMon13]	[MKMZ17, **BKMMZ17**]	[SRF16,HWJ17]	[Reeves17,GML18+]
Multi-layer	[MKMZ17]	[MKMZ17]	[FRS18]	[Reeves17,GML18+]

- [Reeves17]: Reeves, "Additivity of Information in Multilayer Networks via Additive Gaussian Noise Transforms"
  - Postulates SE for ML-VAMP and rigorously proves this for Gaussian case
- [GML18+] Gabrié, Manoel, Luneau, Barbier, Macris, Krzakala, Zdeborová. "Entropy and mutual information in models of deep neural networks." *2018:*
  - Proves multi-layer model rigorously for large class of matrices and L=2 layers

Outline

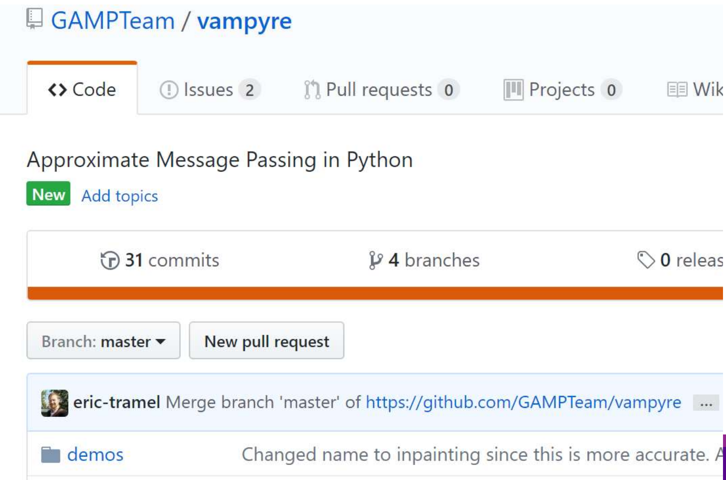
- AMP and Compressed Sensing
- Proximal Operators and ISTA
- State Evolution for AMP
- Bayes Denoising, Optimality and the Replica Method
- Belief Propagation and Factor Graphs
- AMP Derivation from Belief Propagation
- Convergence, Fixed Points and Stability
- Extensions: Vector AMP
- Thoughts on What is Next

Summary and Challenges

- Benefits of AMP
  - Enables rigorous analysis of complex inference problems in random settings
  - Computationally tractable
  - Identifies hard and easy regimes. Optimality guarantees
  - Can be extended to many complex problems
- Algorithmic issues: Still unstable. Requires damping, other tweaks
- Many models unsolved
  - Deep network model today covers inference, not learning
  - Can AMP understand learning multi-layer networks
  - Other key algorithms: VAE, GANs, …

Vampyre

- A new python package
- Thanks to Eric Tramel and others
- Modular, flexible, …
- Try it out!



Multi-Layer Perceptron Inpainting with MNIST

In the MLP demo, we saw how to use the multi-layer VAMP (ML-VAMP) method for der perceptron. We illustrated the method on synthetic data generated from a random MLP r with the MNIST data. Specifically, we consider the problem of estimating an MNIST digit ir form,

$$y = Ax,$$

where A is a sub-sampling operation. The sub-sampling operation outputs a subset of th occuluded area. This problem of reconstructing an image x with a portion of the imag requires a prior on the image. In this demo, we will use an MLP generative model for that p

Importing the Package

We first import the `vampyre` and other packages as in the sparse linear inverse demo.

```
# Add the vampyre path to the system path
import os
import sys
vp_path = os.path.abspath('../../')
if not vp_path in sys.path:
    sys.path.append(vp_path)
import vampyre as vp

# Load the other packages
import numpy as np
import matplotlib
```

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