Message passing and approximate message passing

Arian Maleki

Columbia University

What is the problem?

Given pdf $\mu(x_1, x_2, \dots, x_n)$ we are interested in

- $\arg \max_{x_1, x_2, \dots, x_n} \mu(x_1, x_2, \dots, x_n)$
- Calculating marginal pdf $\mu_i(x_i)$
- Calculating joint distribution $\mu_S(x_S)$ for $S \subset \{1, 2, \ldots, n\}$

These problems are important because

- Many inference problems are in these forms
- Many applications in image procession, communication, machine learning, signal processing

This talk: Marginalizing distribution

Most tools are applied to other problems

This talk: marginalization

Problem: Given pdf $\mu(x_1, x_2, \ldots, x_n)$ find $\mu_i(x_i)$

• Simplification: all x_j 's are binary random variables

Is it difficult?

- Yes. No polynomial time algorithm
- ▶ Complexity of variable elimination: 2ⁿ⁻¹

Solution:

- ▶ No "good solution" for "generic μ "
- Consider structured μ

Structured μ

Problem: Given pdf $\mu(x_1, x_2, \dots, x_n)$ find $\mu_i(x_i)$

Simplification: all x_j's are binary random variables

Example 1: x_1, x_2, \ldots, x_n are independent

- Easy marginalization
- Not interesting

Example 2: Independent subsets

$$\mu(x_1, x_2, \dots, x_n) = \mu'_1(x_1, \dots, x_k)\mu'_2(x_{k+1}, \dots, x_n)$$

- More interesting and less easy
- Complexity still exponential in terms of size of subsets
- Does not cover many interesting cases

Structured μ :Cont'd

Problem: Given pdf $\mu(x_1, x_2, \dots, x_n)$ find $\mu_i(x_i)$

• Simplification: all x_j 's are binary random variables

Example 3: more interesting structure:

$$\mu(x_1, x_2, \dots, x_n) = \mu'_1(x_{S_1})\mu'_2(x_{S_2})\dots\mu'_\ell(x_{S_\ell})$$

- Unlike independence, $S_i \cap S_j \neq \emptyset$
- Covers many interesting practical problems
- Let $|S_i| \ll n, \forall i$. Is marginalization easier than a generic μ ?

o Not clear!! We introduce factor graph to address this question

Factor graph

Slight generalization

$$\mu(x_1, x_2, \dots, x_n) = \frac{1}{Z} \prod_{a \in F} \psi_a(x_{S_a})$$

- $\psi_a: \{0,1\}^{|S_a|} \to \mathbb{R}^+$ not necessarily pdf
- Z: normalizing constant. Called "partition function"
- $\psi_a(x_{S_a})$: factors

Factor graph:

- ► Variable node: n nodes corresponding to x₁, x₂,..., x_n
- Function node: |F| nodes corresponding to $\psi_a(x_{S_1}), \psi_b(x_{S_2}), \ldots$
- Edge between a and variable node i iff $x_i \in S_a$



Factor graph Cont'd

$$\mu(x_1, x_2, \dots, x_n) = \frac{1}{Z} \prod_{a \in F} \psi_a(x_{S_a})$$

Factor graph:

- ► Variable node: n nodes corresponding to x₁, x₂,..., x_n
- ► Function node: F nodes corresponding to ψ_a(x_{S1}), ψ_b(x_{S2}),...
- Edge between a and variable node i iff $x_i \in S_a$

Some notation:

• ∂a : neighbors of function node a:

$$\partial a = \{i : x_i \in S_a\}.$$

• ∂i : neighbors of variable node i

$$\partial i = \{ b \in F : i \in S_b \}.$$



Factor graph example

$$\mu(x_1, x_2, x_3) = \frac{1}{Z} \psi_a(x_1, x_2) \psi_b(x_2, x_3)$$

Some notation:

• ∂a : neighbors of function node a:

$$\partial a = \{1, 2\}$$
$$\partial b = \{2, 3\}$$

• ∂i : neighbors of variable node i

$$\partial 1 = \{a\}$$
$$\partial 2 = \{a, b\}$$



Factor graphs simplifies understanding structures

- Independence: graph has disconnected pieces
- Tree graphs: Easy marginalization
- Loops (specially short loops): generally make the problem more complicated



Marginalization on tree structured graphs

Tree: Graph with no loops

- Marginalization by variable elimination is efficient on such graphs (distributions)
 - \circ Linear in n
 - o Exponential in size of factors
- Proof: on the board



Summary of variable elimination on trees

Notation

•
$$\mu(x_1, x_2, \dots, x_n) = \prod_{a \in F} \psi_a(x_{\partial a})$$

- $\mu_{j \to a}$: belief from variable node j to factor a
- $\hat{\mu}_{a \to j}$: belief from factor node a to variable j

We also have

$$\mu_{a \to j}(x_j) = \sum_{\{x_j : j \in \partial a \setminus j\}} \psi_a(x_{\partial a}) \prod_{\ell \in \partial a \setminus j} \hat{\mu}_{\ell \to a}(x_\ell)$$
$$\hat{\mu}_{j \to a}(x_j) = \prod_{b \in \partial j \setminus a} \mu_{b \to j}(x_j)$$



Belief propagation algorithm on trees

Based on variable elimination on trees consider iterative algorithm:

$$\nu_{a \to j}^{t+1}(x_j) = \sum_{\{x_j : j \in \partial a \setminus j\}} \psi_a(x_{\partial a}) \prod_{\ell \in \partial a \setminus j} \hat{\nu}_{\ell \to a}^t(x_\ell)$$
$$\hat{\nu}_{j \to a}^{t+1}(x_j) = \prod_{b \in \partial j \setminus a} \nu_{b \to j}^t(x_j)$$

- $\blacktriangleright \ \nu_{a \rightarrow j}^t \ \text{and} \ \hat{\nu}_{j \rightarrow a}^t$ are beliefs of nodes at time t
- Each node propagates its belief to other nodes

Hope: Converge to a "good" fixed point

$$\nu_{b \to j}^{t}(x_j) \underset{t \to \infty}{\to} \mu_{b \to j}(x_j)$$
$$\hat{\nu}_{j \to b}^{t}(x_j) \underset{t \to \infty}{\to} \mu_{j \to b}(x_j)$$



Belief propagation algorithm on trees

Belief propagation:

$$\nu_{a \to j}^{t+1}(x_j) = \sum_{\{x_j : j \in \partial a \setminus j\}} \psi_a(x_{\partial a}) \prod_{\ell \in \partial a \setminus j} \hat{\nu}_{\ell \to a}^t(x_\ell)$$
$$\hat{\nu}_{j \to a}^{t+1}(x_j) = \prod_{b \in \partial j \setminus a} \nu_{b \to j}^t(x_j)$$

Why BP and not variable elimination?

- On trees: no good reason
- loopy graphs: can be easily applied



Belief propagation algorithm on trees

Belief propagation:

$$\nu_{a \to j}^{t+1}(x_j) = \sum_{\{x_j : j \in \partial a \setminus j\}} \psi_a(x_{\partial a}) \prod_{\ell \in \partial a \setminus j} \hat{\nu}_{\ell \to a}^t(x_\ell)$$
$$\hat{\nu}_{j \to a}^{t+1}(x_j) = \prod_{b \in \partial j \setminus a} \nu_{b \to j}^t(x_j)$$

Lemma: On a tree graph BP converges to the marginal distributions in finite number of iterations, i.e,

$$\nu_{b \to j}^{t}(x_{j}) \xrightarrow[t \to \infty]{} \mu_{b \to j}(x_{j})$$
$$\hat{\nu}_{j \to b}^{t}(x_{j}) \xrightarrow[t \to \infty]{} \mu_{j \to b}(x_{j})$$



Summary of belief propagation on trees

Equivalent to variable elimination

Exact on trees

Converges in finite number of iterations:

2 times the maximum depth of the tree.



Apply belief propagation to loopy graph:

$$\nu_{a \to j}^{t+1}(x_j) = \sum_{\{x_j : j \in \partial a \setminus j\}} \psi_a(x_{\partial a}) \prod_{\ell \in \partial a \setminus j} \hat{\nu}_{\ell \to a}^t(x_\ell)$$
$$\hat{\nu}_{j \to a}^{t+1}(x_j) = \prod_{b \in \partial j \setminus a} \nu_{b \to j}^t(x_j)$$

Wait until the algorithm converges:

• Announce
$$\prod_{a \in \partial j} \nu_{a \to j}^{\infty}(x_j)$$
 as $\mu_j(x_j)$



Challenges for loopy BP

Does not converge necessarily

• Example :

$$\mu(x_1, x_2, x_3) = \mathbb{I}(x_1 \neq x_2)\mathbb{I}(x_2 \neq x_3)\mathbb{I}(x_3 \neq x_1)$$

o $t = 1$ start with $x_1 = 0$
o $t = 2 \Rightarrow x_2 = 1$
o $t = 3 \Rightarrow x_3 = 0$
o $t = 4 \Rightarrow x_4 = 1$

Even if converges, **not** necessarily the marginal distribution

Can have more than one fixed point



In many applications, works really well

- Coding theory
- Machine vision
- compressed sensing

In some cases, loopy BP can be analyzed theoretically



Some theoretical results on loopy BP

BP equations have at least one fixed point

- Proof uses Brouwer's theorem
- Does not necessarily converge to any of the fixed points
- BP is exact on trees

BP is "accurate" for "locally tree like" graphs

Gallager 1963, Luby et al. 2001, Richardson and Urbanke 2001

Several methods exist for verifying correctness of $\ensuremath{\mathsf{BP}}$

- Computation trees
- Dobrushin condition



BP is "accurate" for "locally tree like" graphs

Heuristic: sparse graphs (without many edges) can be "locally tree like"

How to check?

• If $girth(G) = O(\log(n))$

 $\operatorname{girth}(G)$ is the length of the shortest cycle

► Random (*d_v*, *d_c*) graph is locally tree like with high probability



sufficient condition for convergence of BP

Influence of node j on node i:

$$C_{ij} = \sup_{\underline{x},\underline{x'}} \{ \|\mu(x_i \mid x_{V \setminus i,j}) - \mu(x_i \mid x'_{V \setminus i,j})\|_{TV} : x_l = x'_l \ \forall l \neq j \}$$

Intuition: if the influence of the nodes on each other is very small, then oscillations should not occur

Theorem If $\gamma = \sup_i (\sum_j C_{ij}) < 1$, then BP marginals converge to the true marginals.

Summary of BP

Belief propagation:

$$\nu_{a \to j}^{t+1}(x_j) = \sum_{\{x_j : j \in \partial a \setminus j\}} \psi_a(x_{\partial a}) \prod_{\ell \in \partial a \setminus j} \hat{\nu}_{\ell \to a}^t(x_\ell)$$
$$\hat{\nu}_{j \to a}^{t+1}(x_j) = \prod_{b \in \partial j \setminus a} \nu_{b \to j}^t(x_j)$$

Exact on trees

Accurate on locally tree like graphs

No generic proving technique that works on all problems

Successful in many applications, even when we cannot prove convergence



More challenges

What if μ is a pdf on \mathbb{R}^n ?

Extension seems straightforward

$$\nu_{a \to j}^{t+1}(x_j) = \int_{\{x_j : j \in \partial a \setminus j\}} \psi_a(x_{\partial a}) \prod_{\ell \in \partial a \setminus j} \hat{\nu}_{\ell \to a}^t(x_\ell) d\underline{x}$$
$$\hat{\nu}_{j \to a}^{t+1}(x_j) = \prod_{b \in \partial j \setminus a} \nu_{b \to j}^t(x_j)$$

But, calculations become complicated

- Shall discretize the pdf with certain accuracy
- Do lots of numeric multiple integrations

Exception: Gaussian graphical models

$$\mu(\underline{x}) = \frac{\exp(-\underline{x}^t J \underline{x} + c^t \underline{x})}{Z}$$

- All messages become Gaussian
- NOT the focus of this talk

Approximate message passing

Model



- $x_o:$ k-sparse vector in \mathbb{R}^N
- $A: n \times N$ design matrix
- y: measurement vector in \mathbb{R}^n
- w: measurement noise in \mathbb{R}^n

LASSO

Many useful heuristic algorithms:

► Noiseless: ℓ₁-minimization

 $\begin{array}{ll} \underset{x}{\text{minimize}} & \|x\|_1\\ \text{subject to} & y = Ax \end{array}$

$$||x||_1 = \sum_i |x_i|$$

Noisy: LASSO

$$\underset{x}{\text{minimize}} \quad \frac{1}{2} \|y - Ax\|_2^2 + \lambda \|x\|_1$$

convex optimizations

Chen, Donoho, Saunders (96), Tibshirani (96)

LASSO

Many useful heuristic algorithms:

• Noiseless: ℓ_1 -minimization

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minimize
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Algorithmic challenges of sparse recovery

Use convex optimization tools to solve LASSO

Computational complexity:

- interior point method:
 - o generic tools
 - o appropriate for $N<5000\,$
- homotopy methods:
 - o use the structure of the LASSO
 - o appropriate for N < 50000
- First order methods
 - o Low computational complexity per iteration
 - o Require many iterations

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Message passing for LASSO

Define:

$$\mu(\mathrm{d}x) = \frac{1}{Z} e^{-\beta\lambda \|x\|_1 - \frac{\beta}{2} \|y - Ax\|^2} \mathrm{d}x$$

- ► Z: normalization constant
- $\blacktriangleright \ \beta > 0$

As $\beta \to \infty$:

• μ concentrates around solution of LASSO: \hat{x}^{λ}

Marginalize μ to obtain \hat{x}^{λ}

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Marginalize μ to obtain \hat{x}^{λ}

Message passing algorithm

$$\mu(\mathrm{d}x) = \frac{1}{Z} e^{-\beta\lambda \sum_{i} |x_i| - \frac{\beta}{2} \sum_{a} (y_a - (Ax)_a)^2} \mathrm{d}x$$

Belief propagation update rules:

$$\nu_{i \to a}^{t+1}(s_i) \cong e^{-\beta\lambda|s_i|} \prod_{b \neq a} \hat{\nu}_{b \to i}^t(s_i)$$
$$\hat{\nu}_{a \to i}^t(s_i) \cong \int e^{-\frac{\beta}{2}(y_a - (As)_a)^2} \prod_{j \neq i} \mathrm{d}\nu_{j \to a}^t(s_j)$$

Pearl (82)



Issues of message passing algorithm

$$\nu_{i \to a}^{t+1}(s_i) \cong e^{-\beta\lambda|s_i|} \prod_{b \neq a} \hat{\nu}_{b \to i}^t(s_i)$$
$$\hat{\nu}_{a \to i}^t(s_i) \cong \int e^{-\frac{\beta}{2}(y_a - (As)_a)^2} \prod_{j \neq i} \mathrm{d}\nu_{j \to a}^t(s_j)$$

Challenges:

- messages are distributions over real line
- calculation of messages is difficult
 - o Numeric integration
 - o The number of variables in the integral is N-1
- The graph is not "tree like"
 - o No good analysis tools

Challenges for message passing algorithm

$$\nu_{i \to a}^{t+1}(s_i) \cong e^{-\beta\lambda|s_i|} \prod_{b \neq a} \nu_{b \to i}^t(s_i)$$
$$\hat{\nu}_{a \to i}^t(s_i) \cong \int e^{-\frac{\beta}{2}(y_a - (As)_a)^2} \prod_{j \neq i} \mathrm{d}\nu_{j \to a}^t(s_j)$$

Challenges:

- messages are distributions over real line
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- The graph is not "tree like"

Solution:

blessing of dimensionality:

o as $N \to \infty$: $\hat{\nu}_{a \to i}^t(s_i)$ converges to Gaussian

o as $N \to \infty$: $\nu_{i \to a}^t(s_i)$ converges to

$$f_{\beta}(s;x,b) \equiv \frac{1}{z_{\beta}(x,b)} e^{-\beta|s| - \frac{\beta}{2b}(s-x)^2} \,.$$

Challenges for message passing algorithm

$$\nu_{i \to a}^{t+1}(s_i) \cong e^{-\beta\lambda|s_i|} \prod_{b \neq a} \nu_{b \to i}^t(s_i)$$
$$\hat{\nu}_{a \to i}^t(s_i) \cong \int e^{-\frac{\beta}{2}(y_a - (As)_a)^2} \prod_{j \neq i} \mathrm{d}\nu_{j \to a}^t(s_j)$$

Challenges:

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o as
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o as $N \to \infty$: $\nu^t_{i \to a}(s_i)$ converges to
 $f_{\beta}(s; x, b) \equiv \frac{1}{z_{\beta}(x, b)} e^{-\beta|s| - \frac{\beta}{2b}(s-x)^2}$

Simplifying messages for large N

Simplification of $\hat{\nu}_{a \to i}^t(s_i)$

$$\hat{\nu}_{a \to i}^{t}(s_{i}) \cong \int e^{-\frac{\beta}{2}(y_{a} - (As)_{a})^{2}} \prod_{j \neq i} \mathrm{d}\nu_{j \to a}^{t}(s_{j})$$
$$\cong \mathbb{E} \exp\left(-\frac{\beta}{2}(y_{a} - A_{ai}s_{i} - \sum_{j \neq i} A_{aj}s_{j})^{2}\right)$$
$$\cong \mathbb{E} \exp\left(-\frac{\beta}{2}(A_{ai}s_{i} - Z)^{2}\right)$$

 $Z = y_a - \sum_{j \neq i} A_{aj} s_j \xrightarrow{d} W$; W is Gaussian

$$\left|\mathbb{E}h_{s_i}(Z) - \mathbb{E}h_{s_i}(W)\right| \le \frac{C_t''}{N^{1/2}(\hat{\tau}_{a \to i}^t)^{3/2}},$$

Message passing

As $N \to \infty$, $\hat{\nu}_{a \to i}^t$ converges to a Gaussian distribution.

Theorem

Let $x_{j \to a}^t$ and $(\tau_{j \to a}^t / \beta)$ denote the mean and variance of distribution $\nu_{j \to a}^t$. Then there exists a constant C_t' such that

$$\begin{aligned} \sup_{s_i} |\hat{\nu}_{a \to i}^t(s_i) - \hat{\phi}_{a \to i}^t(s_i)| &\leq \frac{C'_t}{N(\hat{\tau}_{a \to i}^t)^3} ,\\ \hat{\phi}_{a \to i}^t(\mathrm{d}s_i) &\equiv \sqrt{\frac{\beta A_{ai}^2}{2\pi \hat{\tau}_{a \to i}^t}} e^{\beta (A_{ai}s_i - z_{a \to i}^t)^2/2\hat{\tau}_{a \to i}^t} \,\mathrm{d}s_i ,\end{aligned}$$

where

$$z_{a \to i}^t \equiv y_a - \sum_{j \neq i} A_{aj} x_{j \to a}^t, \qquad \hat{\tau}_{a \to i}^t \equiv \sum_{j \neq i} A_{aj}^2 \tau_{j \to a}^t.$$

Donoho, M., Montanari (11)

Shape of $\nu_{i \rightarrow a}^{t}$; intuition

Summary

- $\hat{\nu}_{b \to i}^t(s_i) \approx \text{Gaussian}$
- $\nu_{i \to a}^{t+1}(s_i) \cong e^{-\beta\lambda|s_i|} \prod_{b \neq a} \nu_{b \to i}^t(s_i)$

Shape of $\nu_{i \to a}^{t+1}(s_i)$

•
$$\nu_{i \to a}^{t+1}(s_i) \equiv \frac{1}{z_{\beta}(x,b)} e^{-\beta|s| - \frac{\beta}{2b}(s-x)^2}$$

Message passing (cont'd)

Theorem

Suppose that $\hat{\nu}_{a \to i}^t = \hat{\phi}_{a \to i}^t$, with mean $z_{a \to i}^t$ and variance $\hat{\tau}_{a \to i}^t = \hat{\tau}^t$. Then at the next iteration we have

$$|\nu_{i \to a}^{t+1}(s_i) - \phi_{i \to a}^{t+1}(s_i)| < C/n ,$$

$$\phi_{i \to a}^{t+1}(s_i) \equiv \lambda f_{\beta}(\lambda s_i; \lambda \sum_{b \neq a} A_{bi} z_{b \to i}^t, \lambda^2 (1 + \hat{\tau}^t)) ,$$

and

$$f_{\beta}(s;x,b) \equiv \frac{1}{z_{\beta}(x,b)} e^{-\beta|s| - \frac{\beta}{2b}(s-x)^2}$$

Donoho, M., Montanari (11)

Next asymptotic: $\beta \to \infty$

Reminder:

- $x_{j \to a}^t$ mean of $\nu_{j \to a}^t$
- $\blacktriangleright \ z_{a \to i}^t \ \text{mean of} \ \hat{\nu}_{a \to i}^t$
- $\blacktriangleright \ z_{a \to i}^t \equiv y_a \sum_{j \neq i} A_{aj} x_{j \to a}^t$

Can we write $x_{j \rightarrow a}^{t}$ in terms of $z_{a \rightarrow i}^{t}$?

$$x_{j \to a}^t = \frac{1}{z_\beta} \int s_i \mathrm{e}^{-\beta |s_i| - \beta (s_i - \sum_{b \neq a} A_{bi} z_{b \to i}^t)^2}$$

Can be done, but ...

Laplace method simplifies it $(\beta \rightarrow \infty)$

$$x_{j \to a}^t = \eta(\sum_{b \neq a} A_{bi} z_{b \to i}^t).$$

$$\begin{array}{l} x_{j \rightarrow a}^t \, \, \mathrm{mean} \, \, \mathrm{of} \, \, \nu_{j \rightarrow a}^t \\ z_{a \rightarrow i}^t \, \, \mathrm{mean} \, \, \mathrm{of} \, \, \hat{\nu}_{a \rightarrow i}^t \end{array}$$

$$z_{a \to i}^{t} = y_a - \sum_{j \neq i} A_{aj} x_{j \to a}^{t}$$
$$x_{i \to a}^{t+1} = \eta (\sum_{b \neq a} A_{bi} z_{b \to i}^{t}).$$

Comparison of MP and IST



IST









We can further simplify the messages

$$\begin{aligned} x^{t+1} &= & \eta(x^t + A^T z^t; \lambda^t) \\ z^t &= & y - A x^t + \frac{\|x^t\|_0}{n} z^{t-1} \end{aligned}$$

IST versus AMP





AMP:

$$x^{t+1} = \eta(x^t + A^T z^t; \lambda^t)$$

$$z^t = y - A x^t + \frac{1}{n} \|x^t\|_0 z^{t-1}$$



We can predict the performance of AMP at every iteration in asymptotic regime

Idea:

- $x^t + A^T z^t$ can be modeled as signal plus Gaussian noise
- We keep track of noise variance
- I will discuss this part in the "Risk Seminar"