

# **Belief Propagation & Approximations**

# Discrete Tomography

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## Contributors





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# **Discrete Tomography**

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Density 1 Density 2 Density 3

**Tomography** Essentially a reconstruction from linear measurements obtained from a sparse set of projections.

$$\mathbf{y} = F\mathbf{x} + \mathbf{w}$$
 possible noise

**Application** 

Material Sciences > Biology/Medic.

Observation at angle  $\theta$  $\mathbf{y}_{\theta} = \langle F_{\theta}, \mathbf{x} \rangle$ 

# **Binary Tomography**





(512x512) Binary Phantom

**Binary** Simplest case, two possible absorption levels,  $x_i \in \{s_0, s_1\}$ for ease, map signal to  $\{0, 1\}$ and adjust measurements,

$$y_{\mu} = \sum_{i} F_{\mu i} x_{i}$$

$$\downarrow$$

$$y_{\mu}^{b} = \frac{1}{s_{1} - s_{0}} \left( y_{\mu} - s_{0} \sum_{i} F_{\mu i} \right)$$

# **Binary Tomography**

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#### **Reconstruction?**





Leveraging knowledge of image continuity.







Reconstruction

Thresholding

# Variational Approach

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**Goal** Enforce regularity naturally in the optimization.

(Not bootstrapped ex post facto)

e.g. penalize discontinuities in image.

# Variational Approach

## **Total Variation**

Convex approach, regularizing to promote a sparse gradient.  $\mathrm{TV}(\mathbf{x}) = \sum_{i} |\nabla x_i|$ Solve... argmin  $||\mathbf{y} - F\mathbf{x}||_2^2 + \beta TV(\mathbf{x}) + \mathcal{I}_{[0,1]}(\mathbf{x})$  $\mathbf{X}$ Match observations... ...while penalizing discontinuities... ...ensuring proper bounds.

Ex. implementations: gen. forward-backward splitting, FISTA, augmented lagrangian/alternating minimization...



## Probabilistic Construction (Gouillart et al, 2013)

We desire to estimate the posterior...

$$P(\mathbf{x}|\mathbf{y},F) = \frac{1}{Z}P(\mathbf{y}|\mathbf{x},F)P(\mathbf{x})$$

$$= \frac{1}{Z}\prod_{\mu} \left[g\left(y_{\mu} - \sum_{i \in \mu} x_{i}\right)e^{J_{\mu}\sum_{(ij) \in \mu} \delta_{x_{i},x_{j}}}\right]$$
For some intractable formalization...
$$...over the product of factors (measurements/lines)...
$$...and \text{ stochastic output function...}$$

$$AWGN \qquad e^{-\frac{1}{2\sigma^{2}}\left(y_{\mu} - \sum_{i \in \mu} x_{i}\right)^{2}}$$

$$...promote regularity according to some constant.$$$$

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**Goal** A factorized approximation of the posterior allowing for either MAP or MMSE estimation of **x**.

$$Q(\mathbf{x}) = \prod_{i=1}^{N} q(x_i) \approx P(\mathbf{x}|\mathbf{y}, F)$$

**Graphical Representation** Key to constructing a message passing to accomplish this factorization.





Factors along angle  $\psi$ 

 $y_{\mu}$ 



#### Estimate Posterior via BP Use

a graphical interpretation to construct a message passing.

Factor-variable Messages

 $m_{\mu \to i}(x_i)$  $m_{i \to \mu}(x_i)$ 

 $x_5$ 

Variable-variable Messages

 $x_3$ 

 $x_4$ 

 $x_1$ 

 $x_2$ 

$$\eta_{i \to i+1}^{L}(x_i)$$
$$\eta_{i \to i-1}^{R}(x_i)$$

Outgiong messages calculated via *cavity*: product of all incoming *sans* the message coming from the node we are sending to.





Factors along angle  $\psi$ 





Factors along angle  $\psi$ 





Factors along angle  $\psi$ 







Factors along angle  $\psi$ 







Factors along angle  $\psi$ 



## Variables (pixels)



Factors along angle  $\psi$ 







Factors along angle  $\psi$ 







Factors along angle  $\psi$ 



## Variables (pixels)



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Factors along angle  $\psi$ 



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Factors along angle  $\psi$ 





Factors along angle  $\psi$ 





Factors along angle  $\psi$ 





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Factors along angle  $\psi$ 







Factors along angle  $\psi$ 







Factors along angle  $\psi$ 







Factors along angle  $\psi$ 





Factors along angle  $\psi$ 

$$\alpha = 1/10, \sigma/L = 0.006$$

BP





(Gouillart et al, 2013)

(Gouillart et al, 2013)



$$\alpha = 1/10, \sigma/L = 0.006$$



(Gouillart et al, 2013)



(Gouillart et al, 2013)

## From Lines to Lattices...



Why Lines? BP known to be exact on trees. Nice properties!

**However** each line tied to a factor, resulting in many inner BP calculations and a sequential update.

## From Lines to Lattices...



**A Lattice?** A full model of the entire signal that incorporates local correlations. *(related: MRFs)* 



**Caution** Many tight loops, we cannot expect perfection.

#### **Advantages**

- Prior model not tied to the sampling procedure
- Perhaps a more accurate image model
- Adaptable correlation model (edges & weights) that can possibly be trained to exemplars
- Known results from familiar models
- Potentially fewer messages than line model

## From Lines to Lattices...



**An Ising Model** For binary images, we can see that this prior is just a mapping of the square-lattice Ising Model.



$$P(\mathbf{x}) = \frac{1}{\mathcal{Z}} e^{-\mathcal{H}(\mathbf{x})} \qquad x_i \in \pm 1$$
  
$$\mathcal{H}(\mathbf{x}) = \sum_{\langle i,j \rangle} J_{ij} x_i x_j + \sum_i h_i x_i$$
  
Some local biasing  
Edges & correlation weights





 $O(2dN) < O(4NN_{\theta})$  for  $d < N_{\theta}$ 

However, we cannot use the nice <u>Transfer Matrix</u> approach of the linear model.

Already approximate (LBP), why not approximate more?





Passing on Edges



### Passing on Variables (Marginals)





'

#### **MFA** as an approximation of Partition

When applying the MFA, we are approximating the intractable partition (via its *Free Energy*)...

$$\mathcal{F} = -\log \mathcal{Z} = \sum_{x_1 \in \{0,1\}} \sum_{x_2 \in \{0,1\}} \cdots \sum_{x_N \in \{0,1\}} -\mathcal{H}(\mathbf{x})$$

...by minimizing

$$\mathcal{F}^{\mathrm{nmf}} = -\mathcal{S}(\mathbf{m}) - \mathcal{H}(\mathbf{m})$$

$$= \sum_{i} \{m_{i} \ln m_{i} + (1 - m_{i}) \ln(1 - m_{i})\} + \sum_{i} h_{i} m_{i} + \sum_{\langle i,j \rangle} J_{ij} m_{i} m_{j}$$
Promoting greater entropy
$$m_{i} \triangleq \langle x_{i} \rangle_{m_{i}}(x_{i})$$

(more general)



#### **Finding the Factorization**

Factorize lattice by minimizing MFA Free Energy... ... leading to a *fixed point iteration*.

$$m_i^{(t+1)} = \text{sigmoid}(h_i + \sum_j J_{ij} m_j^{(t)})$$
  
$$\therefore m_i^* = \text{sigmoid}(h_i + \sum_j J_{ij} m_j^*)$$

Well-known MFA result leaves much to be desired in terms of accuracy.



#### More moments -> More Accurate

Can use the *Thouless-Anderson-Palmer* (TAP)-type approach, tracking variance, also. Via Pfleka expansion assuming small coupling...

$$\mathcal{F}^{\text{TAP}} = -\mathcal{S}(\mathbf{m}) + \sum_{i} h_{i}m_{i} + \sum_{\langle i,j \rangle} J_{ij}m_{i}m_{j} + \frac{1}{2} \sum_{\langle i,j \rangle} J_{ij}^{2}v_{i}v_{j}$$
$$v_{i} = m_{i} - m_{i}^{2}$$

Which gives the FPI...

$$\therefore m_i^{(t+1)} = \text{sigmoid}(h_i + \sum_j J_{ij} m_j^{(t)} + (0.5 - m_i^{(t-1)}) \sum_j J_{ij}^2 v_i^{(t)})$$



#### **One Step Further**

Can we compute the variable-factor messages on the marginals as well?



### **Approximate Message Passing (AMP)**

Used with great success for Compressed Sensing problems and general inference, as well.

- "Simple" FPI
- Direct application of same TAP approximations (but for real variables) to CS factor graph.

#### **Bringing it Together**

The full iteration including the BI model factorization...

$$\begin{split} V_{\mu}^{t+1} &= \sum_{i} F_{\mu i}^{2} v_{i}^{t} \\ \omega_{\mu}^{t+1} &= \sum_{i} F_{\mu i} a_{i}^{t} - \frac{V_{\mu}^{t+1}}{\Delta + V_{\mu}^{t}} (y_{\mu} - \omega_{\mu}^{t}) \\ (\Sigma_{i}^{t+1})^{2} &= \left[ \sum_{\mu} \frac{F_{\mu i}^{2}}{\Delta + V_{\mu}^{t+1}} \right]^{-1} \\ R_{i}^{t+1} &= a_{i}^{t} + (\Sigma_{i}^{t+1})^{2} \sum_{\mu} F_{\mu i} \frac{(y_{\mu} - \omega_{\mu}^{t+1})}{\Delta + V_{\mu}^{t+1}} \\ h_{i}^{t+1} &= \frac{(R^{t+1} - 0.5)}{(\Sigma_{i}^{t+1})^{2}} \\ a_{i}^{t+1} &= \text{sigmoid}(h_{i}^{t+1} + \sum_{j} J_{ij} a^{t} - (0.5 - a^{t-1}) \sum_{j} J_{ij}^{2} v^{t}) \\ v_{i}^{t+1} &= a^{t+1} - (a^{t+1})^{2} \end{split}$$

#### Standard AMP Iteration



#### **Bringing it Together**

The full iteration including the BI model factorization...

$$\begin{split} V_{\mu}^{t+1} &= \sum_{i} F_{\mu i}^{2} v_{i}^{t} \\ \omega_{\mu}^{t+1} &= \sum_{i} F_{\mu i} a_{i}^{t} - \frac{V_{\mu}^{t+1}}{\Delta + V_{\mu}^{t}} (y_{\mu} - \omega_{\mu}^{t}) \\ (\Sigma_{i}^{t+1})^{2} &= \left[ \sum_{\mu} \frac{F_{\mu i}^{2}}{\Delta + V_{\mu}^{t+1}} \right]^{-1} \\ R_{i}^{t+1} &= a_{i}^{t} + (\Sigma_{i}^{t+1})^{2} \sum_{\mu} F_{\mu i} \frac{(y_{\mu} - \omega_{\mu}^{t+1})}{\Delta + V_{\mu}^{t+1}} \\ R_{i}^{t+1} &= \frac{(R^{t+1} - 0.5)}{(\Sigma_{i}^{t+1})^{2}} \\ a_{i}^{t+1} &= \text{sigmoid}(h_{i}^{t+1} + \sum_{j} J_{ij} a^{t} - (0.5 - a^{t-1}) \sum_{j} J_{ij}^{2} v^{t}) \\ v_{i}^{t+1} &= a^{t+1} - (a^{t+1})^{2} \end{split}$$

Calculate fields from AMP



#### **Bringing it Together**

The full iteration including the BI model factorization...

 $J_{ij}^2 v^t$ )

$$\begin{split} V_{\mu}^{t+1} &= \sum_{i} F_{\mu i}^{2} v_{i}^{t} \\ \omega_{\mu}^{t+1} &= \sum_{i} F_{\mu i} a_{i}^{t} - \frac{V_{\mu}^{t+1}}{\Delta + V_{\mu}^{t}} (y_{\mu} - \omega_{\mu}^{t}) \\ (\Sigma_{i}^{t+1})^{2} &= \left[ \sum_{\mu} \frac{F_{\mu i}^{2}}{\Delta + V_{\mu}^{t+1}} \right]^{-1} \\ R_{i}^{t+1} &= a_{i}^{t} + (\Sigma_{i}^{t+1})^{2} \sum_{\mu} F_{\mu i} \frac{(y_{\mu} - \omega_{\mu}^{t+1})}{\Delta + V_{\mu}^{t+1}} \\ h_{i}^{t+1} &= \frac{(R^{t+1} - 0.5)}{(\Sigma_{i}^{t+1})^{2}} \\ a_{i}^{t+1} &= \text{sigmoid}(h_{i}^{t+1} + \sum_{j} J_{ij} a^{t} - (0.5 - a^{t-1}) \sum_{j} v_{i}^{t+1} \\ v_{i}^{t+1} &= a^{t+1} - (a^{t+1})^{2} \end{split}$$

Update Binary Ising Factorization



Bringing it Together

A full iteration including the BI model factorization...

 $V^{t+1}_{\mu} = \sum_{i} F^2_{\mu i} v^t_i$  $\omega_{\mu}^{t+1} = \sum_{i} F_{\mu i} a_{i}^{t} - \frac{V_{\mu}^{t+1}}{\Delta + V_{\mu}^{t}} (y_{\mu} - \omega_{\mu}^{t})$  $(\Sigma_{i}^{t+1})^{2} = \left[\sum_{\mu} \frac{F_{\mu i}^{2}}{\Delta + V_{\mu}^{t+1}}\right]^{-1}$  $R_i^{t+1} = a_i^t + (\Sigma_i^{t+1})^2 \sum_{\mu} F_{\mu i} \frac{(y_\mu - \omega_\mu^{t+1})}{\Delta + V_\mu^{t+1}}$  $h_i^{t+1} = \frac{(R^{t+1} - 0.5)}{(\Sigma_i^{t+1})^2}$  $a_i^{t+1} = \text{sigmoid}(h_i^{t+1} + \sum_j J_{ij}a^t - (0.5 - a^{t-1})\sum_j J_{ij}^2 v^t)$  $v_i^{t+1} = a^{t+1} - (a^{t+1})^2$ 

Repeat until some criterion met, like

- Uncertainty
- Residual
- Convergence of factorization



## TAP-BI + AMP



### **Bringing it Together**

A full iteration including the BI model factorization...

$$\begin{split} V_{\mu}^{t+1} &= \sum_{i} F_{\mu i}^{2} v_{i}^{t} & \text{Som} \\ \omega_{\mu}^{t+1} &= \sum_{i} F_{\mu i} a_{i}^{t} - \frac{V_{\mu}^{t+1}}{\Delta + V_{\mu}^{t}} (y_{\mu} - \omega_{\mu}^{t}) & \text{impr} \\ (\Sigma_{i}^{t+1})^{2} &= \left[ \sum_{\mu} \frac{F_{\mu i}^{2}}{\Delta + V_{\mu}^{t+1}} \right]^{-1} & \Delta^{t} \\ R_{i}^{t+1} &= a_{i}^{t} + (\Sigma_{i}^{t+1})^{2} \sum_{\mu} F_{\mu i} \frac{(y_{\mu} - \omega_{\mu}^{t+1})}{\Delta + V_{\mu}^{t+1}} \\ h_{i}^{t+1} &= \frac{(R^{t+1} - 0.5)}{(\Sigma_{i}^{t+1})^{2}} \\ a_{i}^{t+1} &= \text{sigmoid}(h_{i}^{t+1} + \sum_{j} J_{ij} a^{t} - (0.5 - a^{t-1}) \sum_{j} J_{ij}^{2} v^{t}) \\ v_{i}^{t+1} &= a^{t+1} - (a^{t+1})^{2} \end{split}$$

**Some Nuance** One can update noise variance to improve convergence...

$$\Delta^t = \frac{1}{M} ||\mathbf{y} - F\mathbf{a}^t||_2^2$$

# ENS

## **Bringing it Together**

A full iteration including the BI model factorization...

$$\begin{split} V_{\mu}^{t+1} &= \sum_{i} F_{\mu i}^{2} v_{i}^{t} \\ \omega_{\mu}^{t+1} &= \sum_{i} F_{\mu i} a_{i}^{t} - \frac{V_{\mu}^{t+1}}{\Delta + V_{\mu}^{t}} (y_{\mu} - \omega_{\mu}^{t}) \\ (\Sigma_{i}^{t+1})^{2} &= \left[ \sum_{\mu} \frac{F_{\mu i}^{2}}{\Delta + V_{\mu}^{t+1}} \right]^{-1} \\ R_{i}^{t+1} &= a_{i}^{t} + (\Sigma_{i}^{t+1})^{2} \sum_{\mu} F_{\mu i} \frac{(y_{\mu} - \omega_{\mu}^{t+1})}{\Delta + V_{\mu}^{t+1}} \\ h_{i}^{t+1} &= \frac{(R^{t+1} - 0.5)}{(\Sigma_{i}^{t+1})^{2}} \\ a_{i}^{t+1} &= \text{sigmoid}(h_{i}^{t+1} + \sum_{j} J_{ij} a^{t} - (0.5 - a^{t-1}) \sum_{\mu} V_{i}^{t+1} \\ v_{i}^{t+1} &= a^{t+1} - (a^{t+1})^{2} \end{split}$$

# **Some Nuance** Also, one can update the coupling strength...

$$J_{ij}^{t} \triangleq \eta^{t} E_{ij}$$
$$\eta^{t+1} = \frac{1}{N} \sum_{\langle i,j \rangle} J_{i,j}^{t} a_{i}^{t} a_{j}^{t}$$



# ENS

## **Bringing it Together**

A full iteration including the BI model factorization...

$$\begin{split} V_{\mu}^{t+1} &= \sum_{i} F_{\mu i}^{2} v_{i}^{t} & \text{Som} \\ \omega_{\mu}^{t+1} &= \sum_{i} F_{\mu i} a_{i}^{t} - \frac{V_{\mu}^{t+1}}{\Delta + V_{\mu}^{t}} (y_{\mu} - \omega_{\mu}^{t}) & \text{be n} \\ (\Sigma_{i}^{t+1})^{2} &= \left[ \sum_{\mu} \frac{F_{\mu i}^{2}}{\Delta + V_{\mu}^{t+1}} \right]^{-1} & a^{t} \\ R_{i}^{t+1} &= a_{i}^{t} + (\Sigma_{i}^{t+1})^{2} \sum_{\mu} F_{\mu i} \frac{(y_{\mu} - \omega_{\mu}^{t+1})}{\Delta + V_{\mu}^{t+1}} \\ h_{i}^{t+1} &= \frac{(R^{t+1} - 0.5)}{(\Sigma_{i}^{t+1})^{2}} \\ a_{i}^{t+1} &= \operatorname{sigmoid}(h_{i}^{t+1} + \sum_{j} J_{ij} a^{t} - (0.5 - a^{t-1}) \sum_{j} J_{ij}^{2} v^{t}) \\ v_{i}^{t+1} &= a^{t+1} - (a^{t+1})^{2} \end{split}$$

**Some Nuance** Damping can be necessary...

$$a^{t+1} = \beta a^t + (1 - \beta)a^{t+1}$$

## A Small Experiment...

## Target Image



256



#### **Parameters**

$$\epsilon = \Delta/L \in [10^{-2}, 10^{-3}]$$
  
 $\alpha = M/N = N_{\theta}/L \in (0, 0.25]$   
 $d = 8$ 

#### **Small Noise Variance**





#### Large Noise Variance





# Looking Forward

# ENS

## Much work to do...

- What are the effects of learning free parameters?
  - Is there a better update scheme for these?
- Optimal stopping criterion?
- How to choose damping? Adaptive scheme based on free energy?
- Will these changes help high-noise performance?

# Looking Forward



### Much work to do...

• Extension to Potts...some preliminary work applied to limited-angle electron tomography



Au Bipyramid



# Looking Forward

# ENS

## Much work to do...

• Extension to Potts...some preliminary work applied to limited-angle analytic electron tomography



Carbon



Cobalt



Oxygen







## **Questions?**

## **Thanks!**

## Scratch



