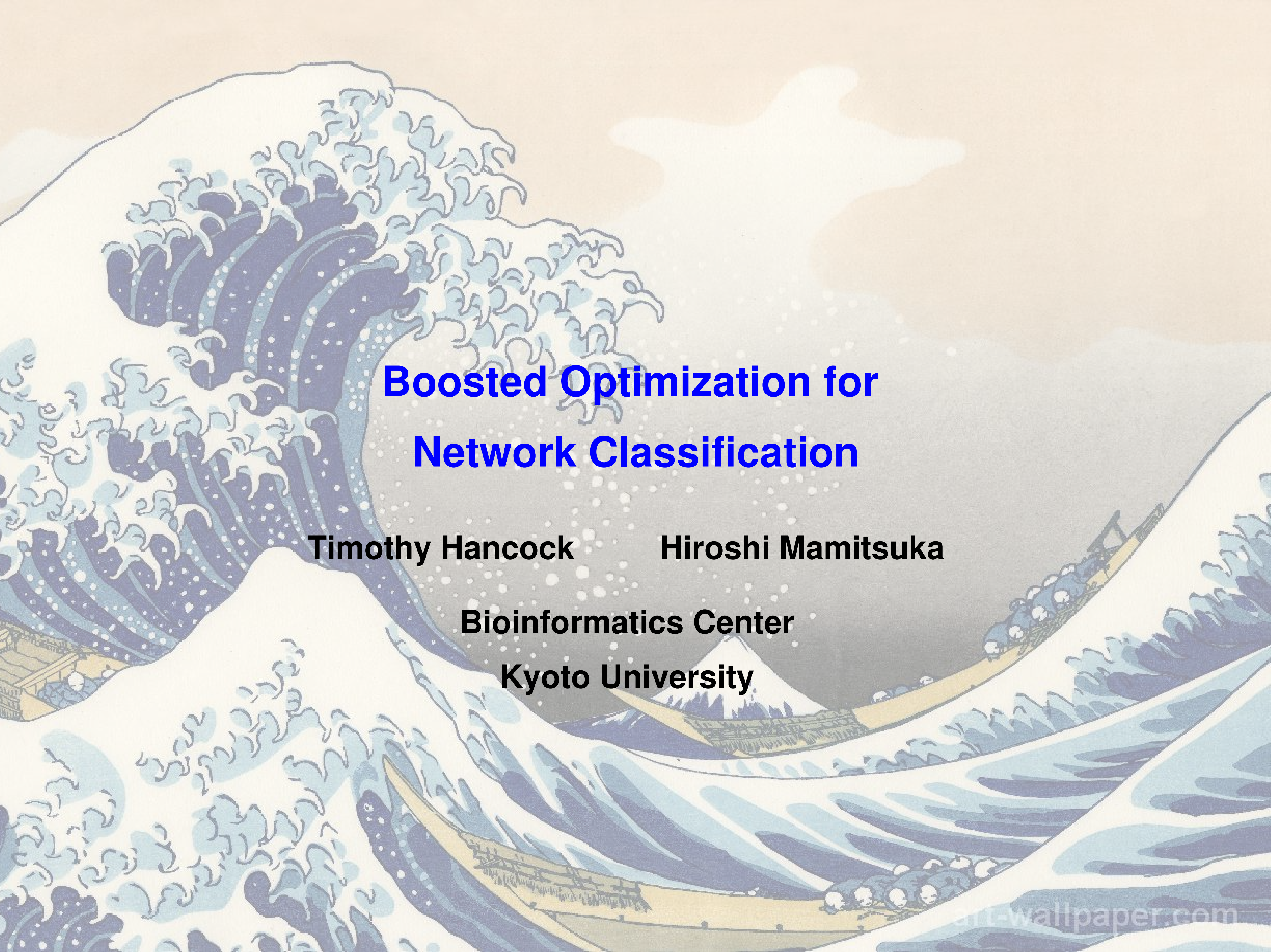

Boosted Optimization for Network Classification

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Motivation

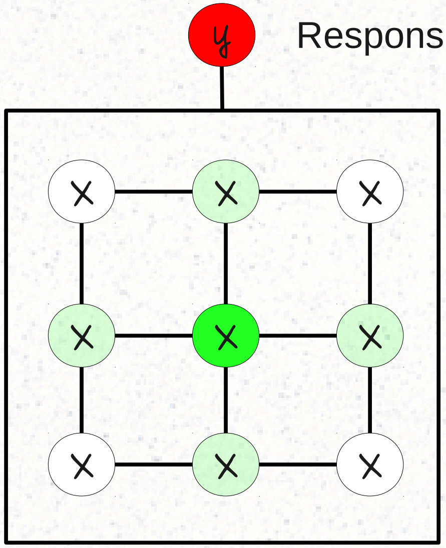
We want to construct a classifier that has good performance where the predictor variables have a known network structure.

For Example:

x strongly classifies y

x have edges with x and are also likely to have a strong relationship with y

The relationship between y and x is unclear and could be obscured by noise.



Response Variable

Predictor variables organized into a known network structure

- Feature selection or regularized methods (lasso etc.) focus on sparsity and may just pick x and some of its neighbors x .
    - This could lead to very sparse graph features being used to represent the entire network.

Can we use the known network structure to resolve the relationship between x and y and improve classification performance?

Outline

1. Problem Setup

I. Network classifiers and logistic regression

II. Logistic regression and exponential loss

III. Network classifiers as an ensemble of factors

2. Methods

I. Boosting

II. Expectation Propagation

III. Boosted Expectation Propagation (BEP)

IV. Message Passing

V. Boosted Message Passing (BMP)

VI. BEP vs BMP

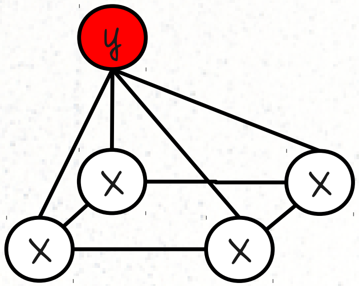
VII. Convergence & Complexity

3. Experiments

4. Summary & Conclusions

Network Classifiers and Logistic Regression

- The link between network classifiers and logistic regression is well established (Friedman, 1997)



- Each predictor variable is a node: $\beta_k x_k$
- Each edge is an interaction effect: $\beta_{km} x_k x_m$
- β are the logistic regression coefficients
- All nodes have an edge with a binary response: $y = [-1, 1]$
- The probability for classifying a binary response is:

$$P(y=1|X) = \frac{e^{F(X)}}{1+e^{F(X)}}$$

- Where $F(X)$ is a linear combination of node and edge terms:

$$F(X) = \sum_k \left(\beta_k x_k + \sum_{m \in ne(x_k)} \beta_{km} x_k x_m \right)$$

Logistic Regression and Exponential Loss

- Optimizing the performance of a logistic regression can be seen as maximizing an exponential potential function.

$$P(y=1|X)=\frac{e^{F(X)}}{1+e^{F(X)}} \qquad \frac{P(y=1|X)}{1-P(y=1|X)}=e^{F(X)}$$

- Increasing $F(X)$ in the direction of y, will optimize classification performance.
- Equivalently, as $y = [-1,1]$ we could minimize the exponential loss:

$$\min\left\{e^{-yF(X)}\right\}$$

- This link between minimizing the exponential loss and maximizing the performance of a logistic regression has been observed with boosted learning (Friedman et al. , 2000).

Network Classifier as an Ensemble of Factors

Consider a factorization of our network classifier to minimize the exponential loss,

$$e^{-yF(X)} = \prod_k e^{-y\left(\beta_k x_k + \sum_{m \in ne(x_k)} \beta_{km} x_k x_m\right)} = \prod_k e^{-y f_k(x_k, ne(x_k), \beta_k)}$$

- The exponential loss is minimized when f_k is maximized in the direction of y. ($y = [-1,1]$)
- Each f_k can be interpreted an individual classifier.
- Optimizing a linear combination of classifiers to minimize an exponential loss is similar to boosting.
    - Except the structure of all ensemble members is specified in advance and represents local potential functions of a known network.

Can we use the known network structure to estimate each classifier f_k which minimizes the exponential loss over the whole network?

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Boosting

- Boosting constructs a linear combination $F_M(X)$ through a stage-wise addition of individual classifiers $f_m(X)$:

$$F_M(X) = \sum_{m=1}^{M} c_m f_m(X)$$

where each new classifier $f_m(X)$ found through minimization of an exponential loss:

$$\underset{c_m}{\operatorname{argmin}} \left\{ e^{-y(F_{m-1}(X)+c_m f_m(X))} \right\} \quad = \quad \underset{c_m}{\operatorname{argmin}} \left\{ w_{m-1} e^{-y c_m f_m(X)} \right\}$$

- The weights at each iteration w_{m-1} are the errors of the current ensemble $F_{M-1}(X)$.

- The boosted coefficients c_m weight the importance of each newly added model $f_m(X)$ to the entire ensemble:

$$e_m = E_{w_{m-1}}[1_{y \neq \hat{f}_m(X)}] \text{ and } c_m = \frac{1}{2} \log \frac{1-e_m}{e_m}$$

Network Inference

Message Passing and Expectation Propagation are network inference algorithms that work on factor graphs:

- Starting from a factorization of pairwise loss functions:

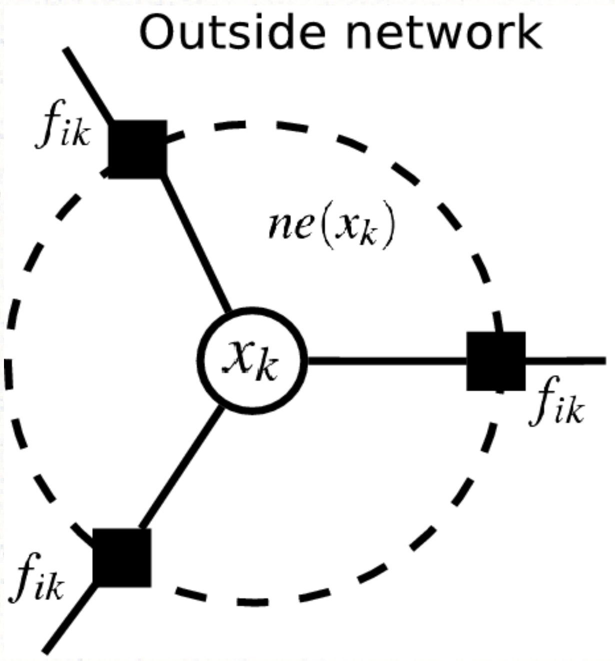
$$f_{ik} = f_{ik}(x_k, x_i) = e^{-y(\beta_k x_k + \beta_{ik} x_k x_i)}$$

- The contribution of x_k to the whole network is:

$$q_k(x_k) = \prod_{i \in ne(x_k)} f_{ik}$$

- The entire network can be re-written as:

$$p(X) = \prod_k q_k(x_k) = \prod_k \prod_{i \in ne(x_k)} f_{ik}$$



From this factorization we can directly use Expectation Propagation or Message Passing algorithms to optimize the performance of our network classifier.

Expectation Propagation (EP)

Expectation Propagation (EP) minimizes the Kullback-Leibler divergence of a factorized distribution by iteratively refining the estimates of each factor (Minka, 2001).

Given a factorized distribution: $P(x_1,\ldots,x_m) = \prod_k f_k$

Step 1: Remove the current estimate of f_k

$$\hat{p}(X)^{/f_k} = \hat{p}(X)/\hat{f}_k$$

Step 2: Re-estimate f_k given the the current estimates of all other factors

$$\hat{f}_k = \max\left\{\hat{p}(X)^{/f_k} f_k\right\}$$

Step 3: Insert the new f_k back into the full distribution

$$\hat{p}(X) = Z_k \hat{p}(X)^{/f_k} \hat{f}_k$$

EP on a Network Classifier

If we consider the factorized form of our network classifier:

$$p(X) = \prod_{k} \prod_{i \in ne(x_k)} f_{ik} \quad \text{where} \quad f_{ik} = e^{-y(\beta_i x_i + \beta_{ik} x_i x_k)}$$

We can define an EP algorithm to estimate the classifier parameters β

Step 1: Remove the current estimate of f_{ik}

$$\hat{p}(X)^{/\hat{f}_{ik}} \propto e^{-y\left(F(X) - \hat{f}_{ik}\right)}$$

Step 2: Re-estimate f_{ik} given the current estimates of all other factors

$$\hat{f}_{ik} = \min_{\beta_{ik}} \left\{ \hat{p}(X)^{/\hat{f}_{ik}} e^{-y f_{ik}} \right\}$$

Step 3: Insert the new f_{ik} back into the full distribution

$$\hat{p}(X) \propto \hat{p}(X)^{/\hat{f}_{ik}} e^{-y \hat{f}_{ik}}$$

Step 2 is the minimization of the exponential loss of f_{ik} weighted by the exponential loss of all other factors

Step 2 is analogous to a **Boosted Addition** of f_{ik} to the entire network classifier

Boosted Expectation Propagation (BEP)

Defines a **Boosted update** as the optimization step within an **Expectation Propagation** algorithm:

Step 1: Remove the current estimate of f_{ik}

$$\hat{p}(X)^{/\hat{f}_{ik}} \propto e^{-y(F(X)-\boxed{c_{ik}}\hat{f}_{ik})}$$

Step 2: Re-estimate f_{ik} given the current exponential loss from all other factors

$$\hat{f}_{ik} = \min_{\boxed{c_{ik}}} \{w_{ik}e^{-y\boxed{c_{ik}}f_{ik}}\}$$

Step 3: Insert the new f_{ik} back into the full distribution

$$\hat{p}(X) \propto w_{ik}e^{-y\boxed{c_{ik}}\hat{f}_{ik}}$$

The **boosted update** introduces a new parameter c_{ik} for each f_{ik} which weights the importance of each factor to the network classifier.

Message Passing (MP)

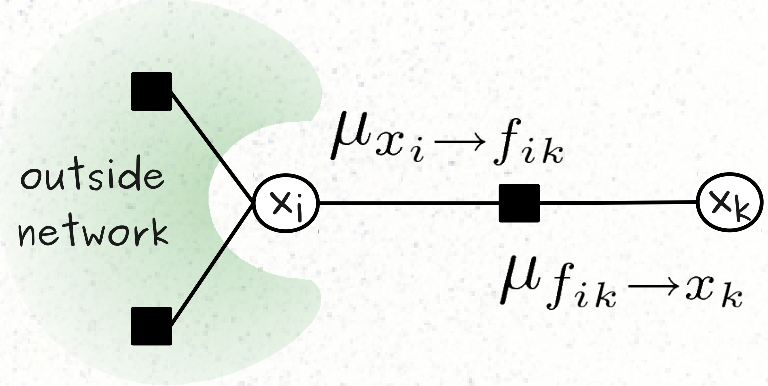
Message Passing algorithms assume that all network information needed to estimate the distribution of node is contained within its immediate neighbors. - We use the max-product algorithm (Kschischang et al., 2001)

Given a factor graph: $P(x_1, \ldots, x_m) = \prod_k f_k$

On a factor graph the max-product algorithm defines 2 type of messages:

1) From a node x_i to a factor f_{ik}:

$$\mu_{x_i \to f_{ik}} = \prod_{\substack{j \in ne(x_i) \\ j \neq k}} \mu_{f_{ji} \to x_i}$$



2) From a factor f_{ik} to a node x_k:

$$\mu_{f_{ik} \to x_k} = \max \left\{ f_{ik} \prod_{\substack{j \in ne(f_{ik}) \\ j \neq k}} \mu_{x_j \to f_{ik}} \right\}$$

MP on a Network Classifier

If we consider the factorized form of our network classifier:

$$p(X) = \prod_{k} \prod_{i \in ne(x_k)} f_{ik} \quad \text{where} \quad f_{ik} = e^{-y(\beta_i x_i + \beta_{ik} x_i x_k)}$$

We can define a max-product algorithm to estimate the classifier parameters β

1) From a node x_i to a factor f_{ik}:

$$\mu_{x_i \to f_{ik}} = \prod_{\substack{j \in ne(x_i) \\ j \neq k}} \mu_{f_{ji} \to x_i}$$

2) From a factor f_{ik} to a node x_k:

$$\boxed{\mu_{f_{ik} \to x_k} = \min \left\{ e^{-y f_{ik}} \prod_{\substack{j \in ne(f_{ik}) \\ j \neq k}} \mu_{x_j \to f_{ik}} \right\}}$$

2) is the minimization the exponential loss of f_{ik} weighted by the exponential loss of the neighboring nodes

Step 2 analogous to a **Boosted Addition** of f_{ik} to the local network structure.

Boosted Message Passing (BMP)

Defines a **Boosted** update as the maximization step within an loopy max-product **Message Passing** algorithm.

1) From a node x_i to a factor f_{ik}:

$$\mu_{x_i \to f_{ik}} = \prod_{\substack{j \in ne(x_i) \\ j \neq i}} \mu_{f_{ji} \to x_i}$$

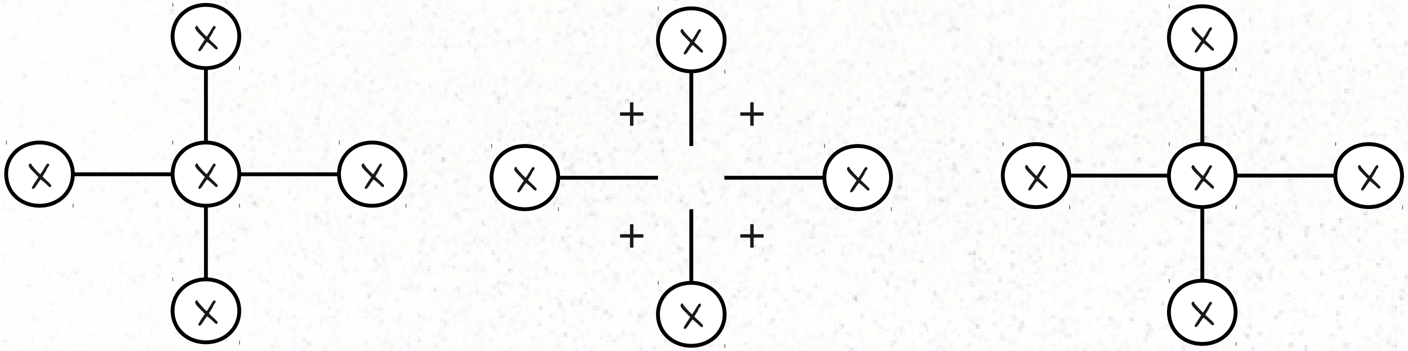
2) From a factor f_{ik} to a node x_k:

$$\mu_{f_{ik} \to x_k} = \min \left\{ e^{-y \boxed{c_{ik}} f_{ik}} \prod_{\substack{j \in ne(f_{ik}) \\ j \neq k}} \mu_{x_j \to f_{ik}} \right\}$$

The **boosted update** introduces a new parameter c_{ik} for each f_{ik} which weights the importance of each factor to the network classifier.

BEP vs BMP

BEP updates each factor based on the error of the entire network:



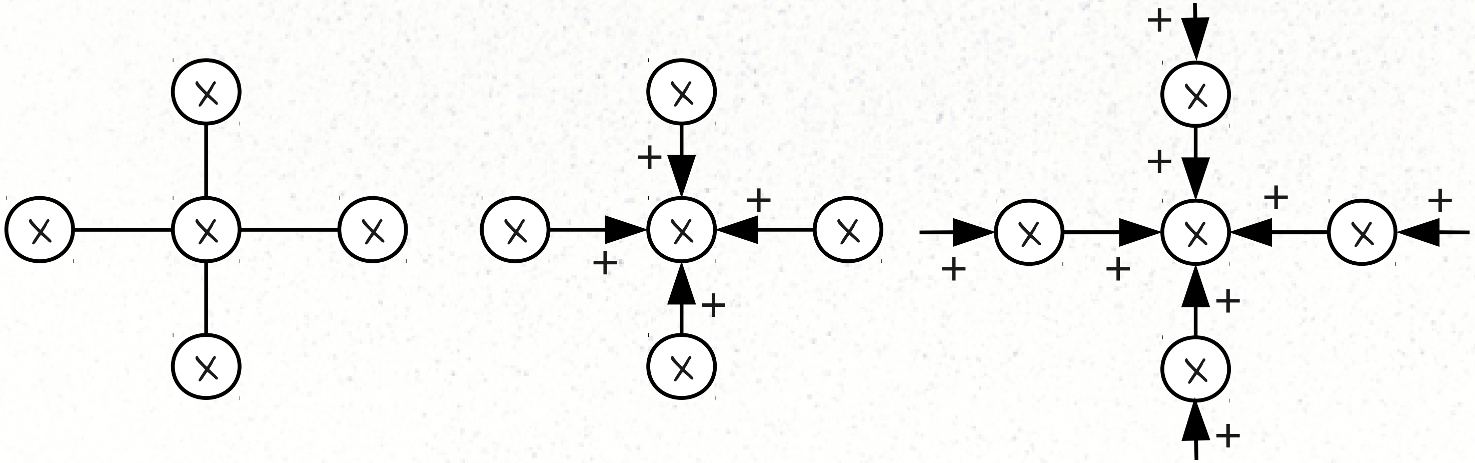
base network

remove each node

re-estimate & re-insert

The network is single ensemble of factors

BMP updates each factor based only on the error within the local network:



base network

1st iteration (estimate and propagate)

2nd iteration (estimate and propagate)

Separate ensembles are built along each edge in both directions

Convergence

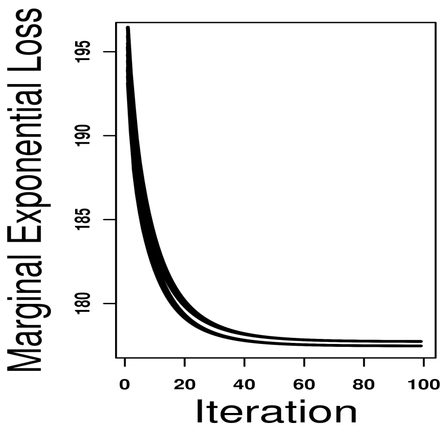
Both MP and EP seek to minimize the Kullback-Leibler divergence. For classification we seek to minimize the Conditional Kullback-Leibler divergence (CKL):

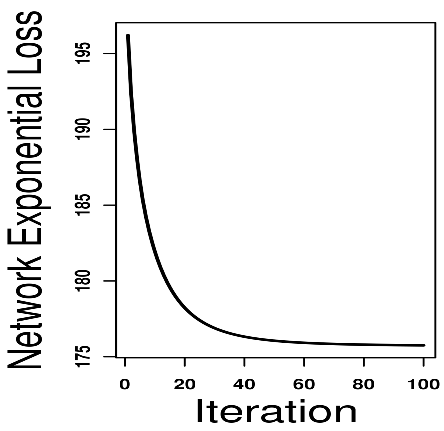
$$CKL(P||Q) = \sum_{y,X} P(X|y) \log \frac{P(X|y)}{Q(X|y)}$$

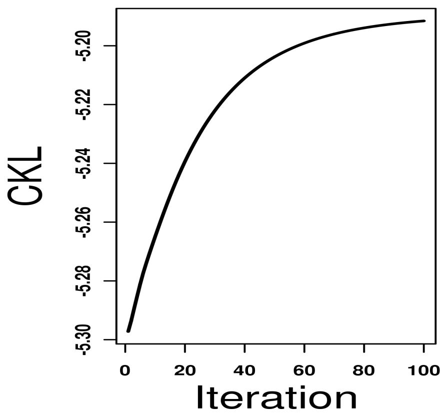
given, $P(X|y) = \frac{1}{Z(X)} \prod_k e^{-yf_k}$ and $Q(X|y) = \prod_k q_k$

Then the CKL is: $\boxed{CKL = -\log Z(X) - \sum_{y,X} yF(X)P(X|y)}$

Boosting only increases f_k linearly, $P(X|y) < 1$ and $Z(X)$ decreases exponentially.







Simulation Experiments

We assess the performance of BEP and BMP to classify a 2D grid structured known exponentially distributed network ($y = 1$):

$$p(X) = \prod_i e^{\theta_i x_i + \sum_{j \in ne(x_i)} \theta_{ij} x_i x_j} \qquad \begin{cases} x_i \in \{-1, 1\} \\ \theta_i \in [-1, 1] \end{cases}$$

embedded within a uniform random noise distribution ($y = -1$).

We define a network strength: $\alpha \in [0.5, 0.75, 1, \ldots, 3]$

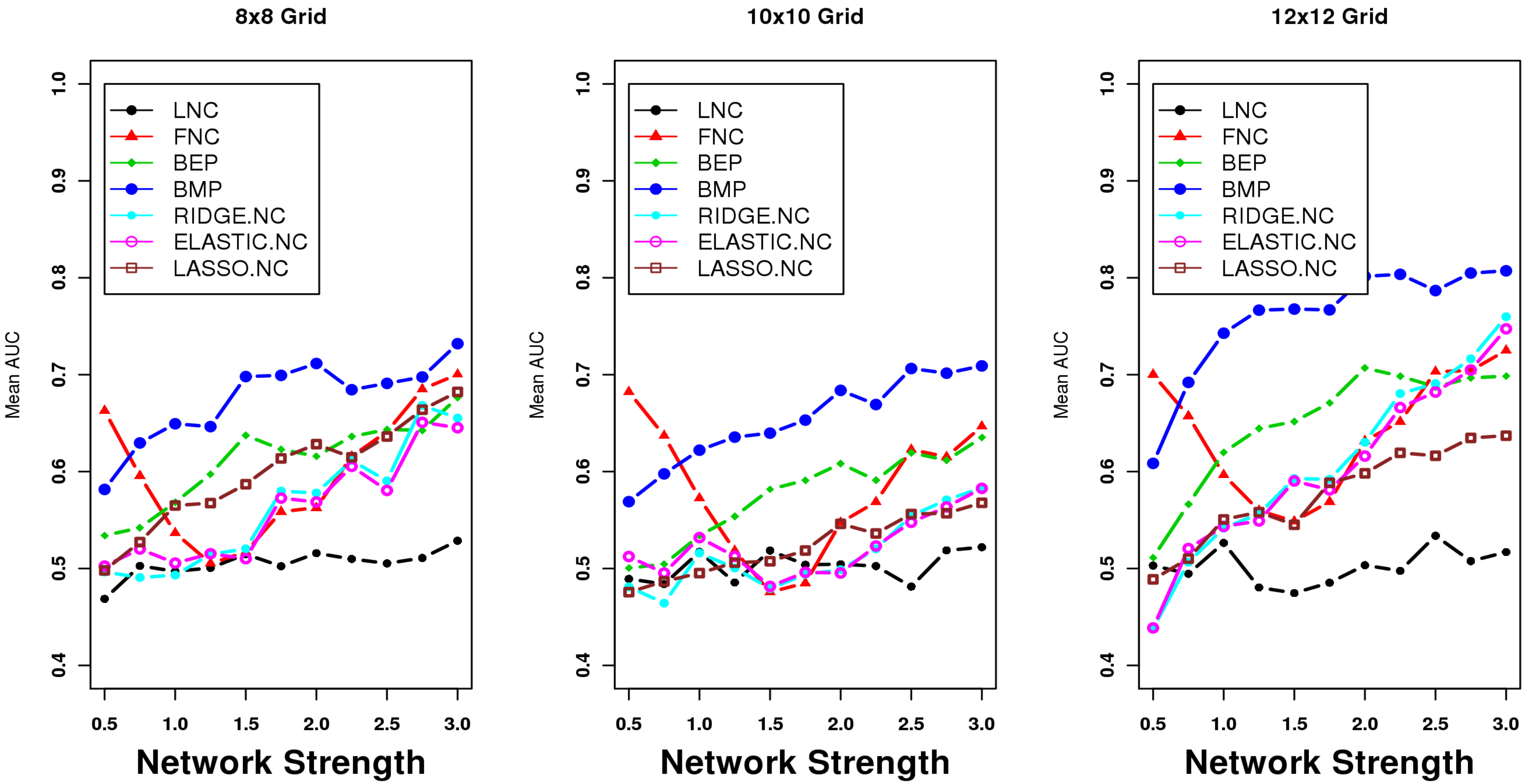
to scale the network coefficients: $\theta_i = \alpha \theta_i$

We compare BEP and BMP on 3 grid sizes (8x8, 10x10, 12x12) with

- Standard logistic regression (LNC)
- Logistic Regression with RIDGE, LASSO and ELASTIC net penalties.
- Simple aggregation over all network factors (FNC)

Using 5x5 fold cross-validation and the area under a ROC curve (AUC).

2D Grid Simulation Results



- BMP performs best
- BEP performance is equivalent to penalized approaches
- As network strength increases all methods will perform around the same.

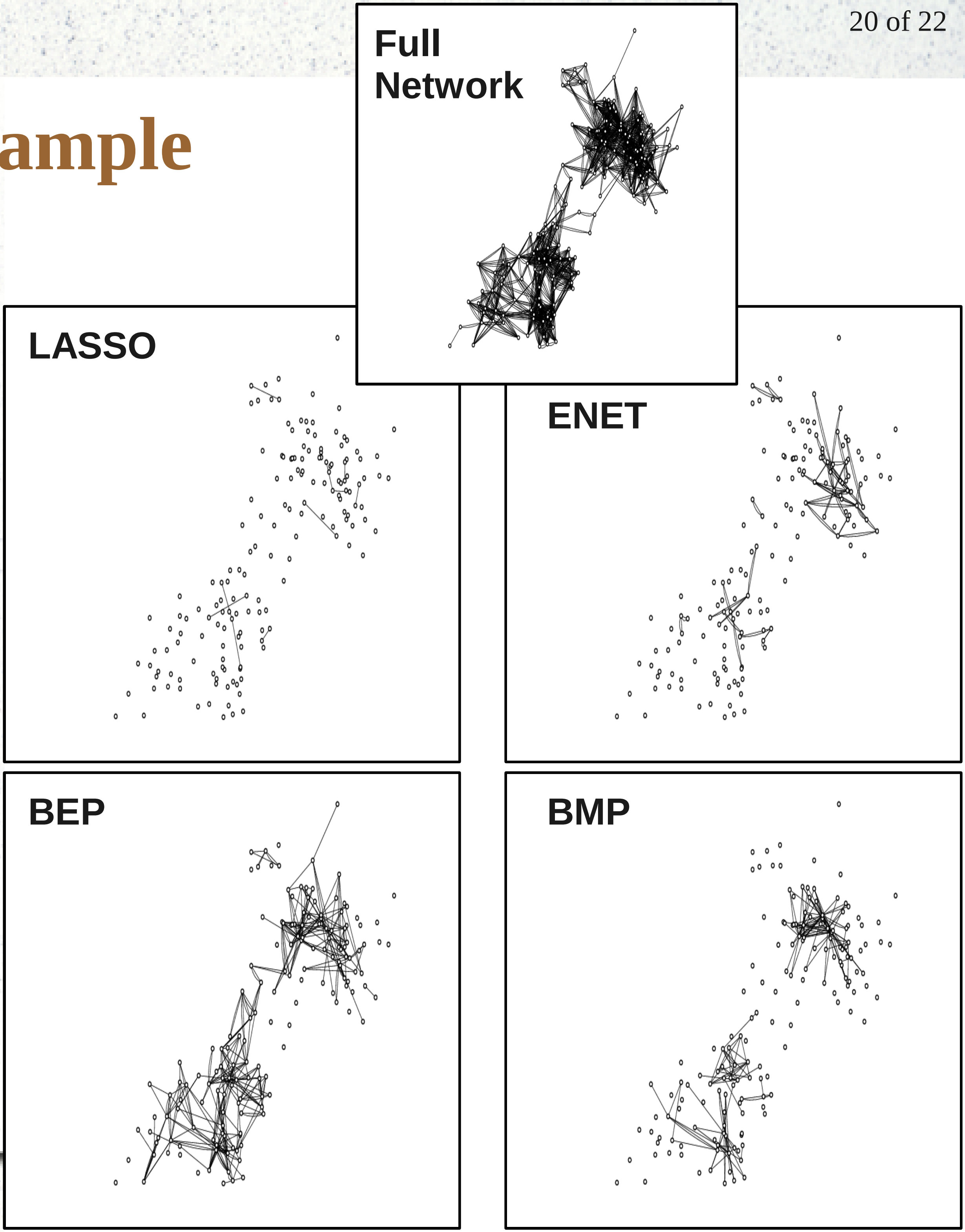
Gene Network Example

KEGG *yeast* carbohydrate metabolism network

203 genes & 1773 interactions

Classify “*heat shock*” specific response from other environmental stresses using the benchmark Gasch microarray data (Gasch et al., 2000).

Model	AUC
RIDGE	0.86 ± 0.028
LASSO	0.865 ± 0.022
ENET	0.88 ± 0.021
BEP	0.87 ± 0.022
BMP	$\mathbf{0.94 \pm 0.013}$



Summary

- We exploit the similarity between logistic regression, boosting and message passing algorithms and propose two novel network classifiers – BEP and BMP.
- BMP is shown to outperform commonly used penalized approaches and BEP shows equivalent performance.
- The results highlight the advantage of explicitly using the known network structure in constructing a classifier.
- BEP and BMP are flexible as they work on a factor graph and can be extended to use topological features of biological networks such as reactions, pathways or GO function information.

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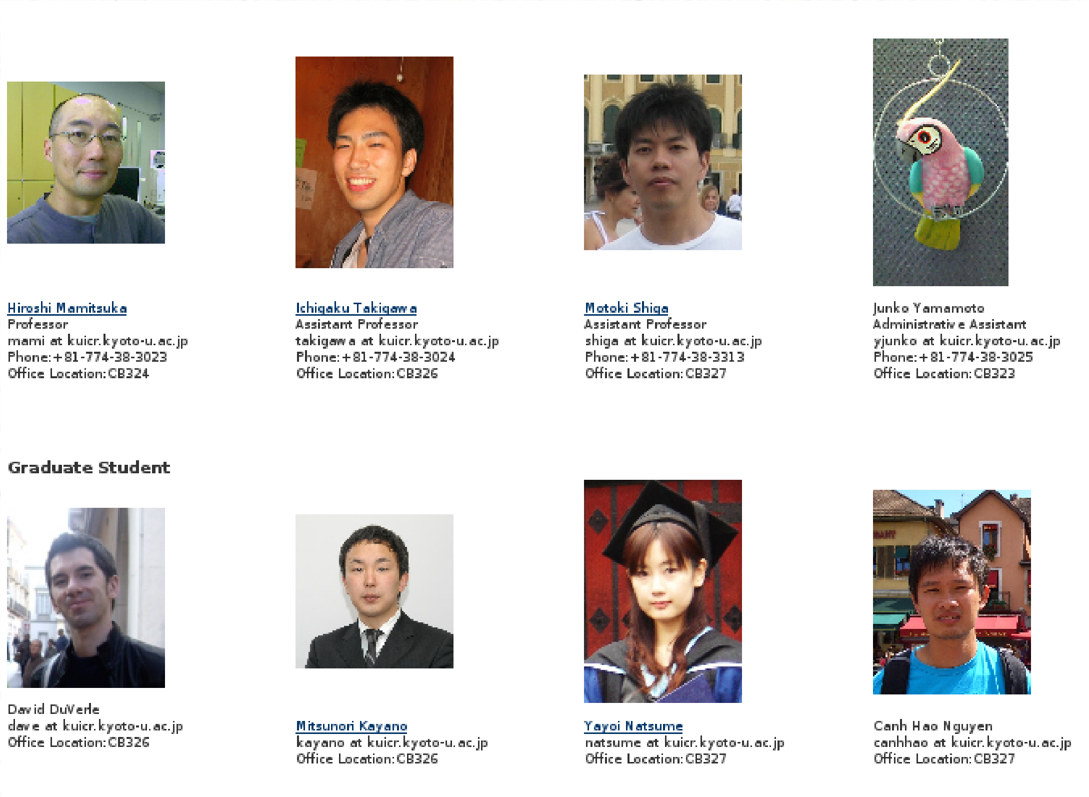

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