Bayesian learning of sparse factor loadings

Magnus Rattray School of Computer Science, University of Manchester

Bayesian Research Kitchen, Ambleside, September 6th 2008

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- Brief overview of popular sparsity priors
- Example application: sparse Bayesian factor analysis for network inference
- Theory for average-case performance with mixture prior
- Theory and MCMC results for different data distributions
- Comparison with L1 prior
- Discussion

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Popular sparsity priors

Sparsity priors tend to be convenient rather than realistic, e.g.

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$$p(w_i) = \mathcal{N}(w_i|0, \lambda_i^{-1})$$

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Mixture

$$p(w_i) = (1 - C)\delta(w_i) + C\mathcal{N}(w_i|0,\lambda^{-1})$$

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Is it OK to not worry about whether these actually fit the data?

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Regulatory network inference Gibbs sampler

Example application: factor analysis for network inference

 $\mathsf{Y} \sim \mathcal{N}(\mathsf{WZ} + oldsymbol{\mu}, oldsymbol{\Psi})$

- $\mathbf{Y} = [y_{in}]$ log-expression of gene *i* in sample *n*
- $Z = [z_{jn}]$ log-concentration (or "activity") of TF j in sample n
- $\mathbf{W} = [w_{ij}]$ factor loading is "effect" of TF j on gene i
 - Model Z as latent variable, since mRNA data may not capture TF protein level/activity, or TFs too weakly expressed
 - For e.g. yeast W roughly 6000×200
 - Various methods for inferring sparse W from Y (reviewed by Pournara and Wernisch, BMC Bioinformatics 2007).

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Regulatory network inference Gibbs sampler

Factor analysis for network inference

$$\mathsf{Y} \sim \mathcal{N}(\mathsf{WZ} + oldsymbol{\mu}, oldsymbol{\Psi})$$

Mixture prior leads to tractable Gibbs sampler

$$p(w_{ij}) = (1 - C_{ij})\delta(w_{ij}) + C_{ij}\mathcal{N}(w_{ij}|0,\lambda^{-1})$$

• Hyper-parameters $C_{ij} \in [0, 1]$ can be obtained from e.g.

- ChIP-chip data
- DNA motifs (Sabatti and James, Bioinformatics 2006)

Or we can estimate (grouped) hyper-parameters by MCMC

Regulatory network inference Gibbs sampler

Gibbs sampler

Write $w_{ij} = x_{ij} b_{ij}$ where $x_{ij} \in \{0,1\}$ and $b_{ij} \sim \mathcal{N}(0,\lambda^{-1})$

$$\begin{array}{rcl} x_{\cdot j} &\sim & p(x_{\cdot j} | \mathbf{X} \setminus x_{\cdot j}, \mathbf{Z}, \mathbf{Y}) & (1) \\ \mathbf{B} &\sim & p(\mathbf{B} | \mathbf{X}, \mathbf{Z}, \mathbf{Y}) & (2) \\ \mathbf{Z} &\sim & p(\mathbf{Z} | \mathbf{X}, \mathbf{B}, \mathbf{Y}) & (3) \end{array}$$

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- Integrate out B before sampling X
- ▶ (2,3) more efficient when X is typically sparse
- Can also sample hyper-parameters C_{ij} and λ if required

Average case theory for sparse Bayesian PCA

$$\mathbf{y}_{n} \sim \mathcal{N}(\mathbf{0}, \sigma^{2}\mathbf{I} + \mathbf{w}\mathbf{w}^{T})$$

$$p(\mathbf{w}|C, \lambda) = \prod_{i=1}^{N} \left[(1-C)\delta(w_{i}) + C\mathcal{N}(w_{i}|0, \lambda^{-1}) \right]$$

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$$\rho(\boldsymbol{w}^*) = \frac{\boldsymbol{w}^* \cdot \boldsymbol{w}^t}{||\boldsymbol{w}^*||||\boldsymbol{w}^t||}$$

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Average case theory for sparse Bayesian PCA

 Similar replica calculation to Uda and Kabashima (J. Phys. Soc. Japan 74, 2005)

$$Z(D) = p(D|C,\lambda) = \int \mathrm{d}\boldsymbol{w} p(\boldsymbol{w}|C,\lambda) \prod_{n=1}^{N} p(\boldsymbol{y}_n|\boldsymbol{w})$$

$$\frac{1}{N} \langle \log Z(D) \rangle_{D, \boldsymbol{w}^{t}} = \frac{1}{N} \lim_{n \to 0} \frac{\partial}{\partial n} \langle Z^{n}(D) \rangle_{D, \boldsymbol{w}^{t}} \\ = \alpha \langle \log p(\boldsymbol{y} | \boldsymbol{w}^{*}(D), C, \lambda) \rangle_{\boldsymbol{y}, D, \boldsymbol{w}^{t}} + \text{entropic terms}$$

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Average case becomes typical for large N due to self-averaging

Standard PCA result Results for sparse PCA (C<1) Results for well-matched data Results for unmatched data L1 prior

Standard PCA result (C=1)

Learning exhibits phase transitions, e.g. (for lpha>1)

$$\rho(w^*) = \theta(\alpha - T^{-2}) \theta\left(\alpha - \frac{\lambda}{NT}\right) \sqrt{\frac{\alpha - T^{-2}}{\alpha + T^{-1}}}$$

where $\theta(x)$ is the step function and

$$T = ||w_t||_{N \to \infty}^2 = NC_t \lambda_t^{-1}$$

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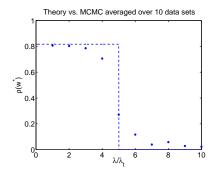
- Consistent with result for Bayesian PCA with spherical prior $p(w) \propto \delta(||w|| 1)$ (Riemann et al. J. Phys. A 1996)
- \blacktriangleright Only new feature is 1st-order transition with increasing λ

Standard PCA result

Results for sparse PCA (C<1) Results for well-matched data Results for unmatched data L1 prior

Standard PCA result (C=1)

 $\lambda_t = N, N = 5000, M = 20000 \ (\alpha = 5)$

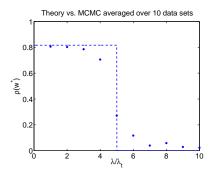


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L1 prior

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Here we will only consider learning away from phase transitions

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Results for sparse PCA (C<1)

▶ We consider two types of data set distribution:

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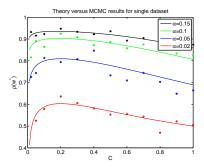
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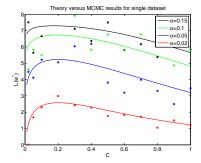
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 - Both give identical performance if sparsity is known

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Results for data distribution (1): $ho(w^*)$ and $\mathcal{L}(w^*)$

 $p(w_i^t) = (1 - C_t)\delta(w_i^t) + C_t \mathcal{N}(w_i^t | 0, \lambda_t^{-1})$ $C_t = 0.2, \lambda = \lambda_t = N/100, M = 200, N = M/\alpha$





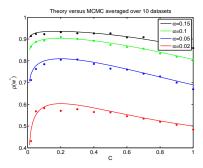
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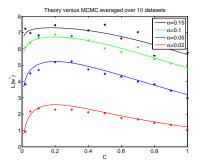
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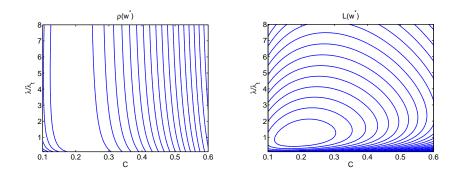
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 $C_t = 0.2, \lambda_t = 20, M = 200, N = 2000 (\alpha = 0.1)$



Bayesian learning of sparse factor loadings

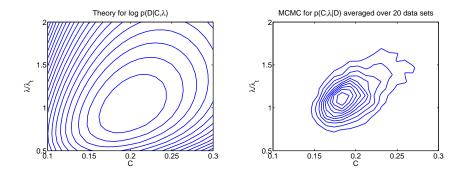
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Bayesian learning of sparse factor loadings

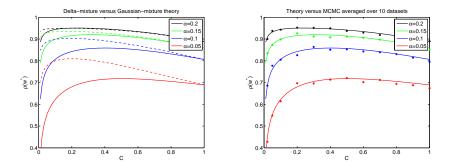
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Standard PCA result Results for sparse PCA (C<1) Results for well-matched data **Results for unmatched data** L1 prior

Results for data distribution (2):
$$\rho(w^*)$$

$$p(w_i^t) = (1 - C_t)\delta(w_i^t) + C_t\delta(w_i^t - \lambda_t^{-1/2}) C_t = 0.2, \lambda = \lambda_t = N/100, M = 200, N = M/\alpha$$



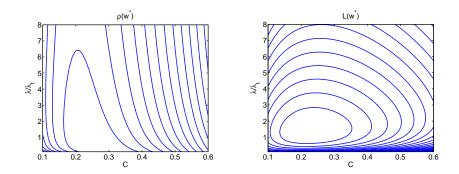
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 $C_t = 0.2, \lambda_t = 10, M = 200, N = 1000 (\alpha = 0.2)$



Bayesian learning of sparse factor loadings

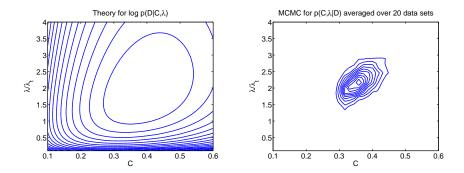
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Is this problem specific to the mixture prior?

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Popular sparsity priors	Standard PCA result
Sparse Bayesian factor analysis	Results for sparse PCA (C<1)
Average case theory	Results for well-matched data
Results	Results for unmatched data
Discussion	L1 prior

Other priors?

- Is this problem specific to the mixture prior?
- Consider the L1 prior (with an additional L2 term),

$$p(w_i) \propto e^{-rac{\lambda_2 w_i^2}{2} - \lambda_1 |w_i|}$$

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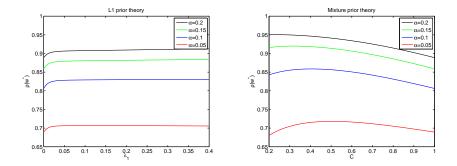
Data distribution (2)

$$\rho(w_i^t) = (1 - C_t)\delta(w_i^t) + C_t\delta(w_i^t - \lambda_t^{-1/2})$$

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L1 prior results: $\rho(w^*)$

$$C_t = 0.2, \lambda_t = N/100, \alpha = M/N$$

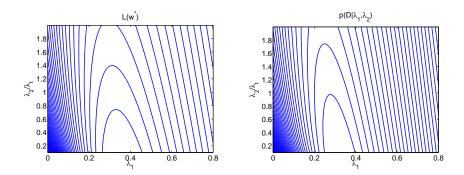


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L1 prior results:
$$ho(D|\lambda_1,\lambda_2)$$
 versus $\mathcal{L}(w^*)$ and $ho(w^*)$

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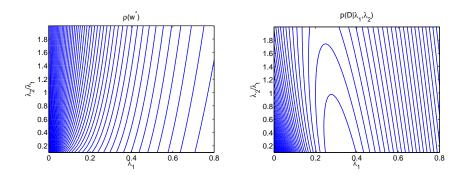


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- Marginal likelihood seems more effective for L1 prior
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- Future work should look at multiple factors
- Assessment of metrics using the full posterior
- Comparison with MAP and ML approaches
- And better priors!

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