FastInf: An Efficient Approximate Inference Library

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Joint work with
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Probabilistic Graphical Models 101

Pr(X₁, ..., Xₙ) = \frac{1}{Z(\Psi)} \prod_{k=1}^{K} \psi_k(C_k)

C_k = \{X_{i_1}, \ldots, X_{i_k}\} : Sets of variables

\Psi = \{\psi_k\}_{k=1}^{K} : The parameterization

Z(\Psi) : The partition function

Pearl 1988
Factor Graphs

\[ Pr(X_1, \ldots, X_n) = \frac{1}{Z(\Psi)} \prod_{k=1}^{K} \psi_k(C_k) \]

\[ C_1 = \{ X_1, X_2, X_3 \} \]
\[ C_2 = \{ X_3, X_4, X_5 \} \]
\[ C_3 = \{ X_5, X_6 \} \]

Frey et al. 2003
Factor Graphs

\[ Pr(X_1, \ldots, X_n) = \frac{1}{Z(\Psi)} \prod_{k=1}^{K} \psi_k(C_k) \]

Frey et al. 2003
Factor Graphs

\[ C_1 = \{X_1, X_2, X_3\} \]

\[
\begin{array}{cccc}
X_1 & X_2 & X_3 & \psi_1(X_3 X_3 X_3) \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 2 \\
0 & 1 & 1 & 1.5 \\
1 & 0 & 0 & 0.2 \\
1 & 0 & 1 & 1.3 \\
1 & 1 & 0 & 1 \\
1 & 1 & 1 & 5 \\
\end{array}
\]

\[ X, X_n) = \frac{1}{Z(\Psi)} \prod_{k=1}^{K} \psi_k(C_k) \]

Frey et al. 2003
Factor Graphs

\[ Pr(X_1, \ldots, X_n) = \frac{1}{Z(\Psi)} \prod_{k=1}^{K} \psi_k(C_k) \]

\[ C_1 = \{X_1, X_2, X_3\} \]
\[ C_2 = \{X_3, X_4, X_5\} \]
\[ C_3 = \{X_5, X_6\} \]

Frey et al. 2003
Example - HMM

\[ Pr(H_1, \ldots, H_n, X_1, \ldots, X_n) = Pr(H_1) \prod_{t=1}^{T} Pr(X_t|H_t) \prod_{t=1}^{T-1} Pr(H_{t+1}|H_t) \]
Example - HMM

\[ C_1 = \{H_1, H_2\} \]
\[ C_2 = \{H_2, H_3\} \]
\[ C_3 = \{H_3, H_4\} \]
\[ C_4 = \{H_4, H_5\} \]

\[ C_5 = \{X_1, H_1\} \]
\[ C_6 = \{X_2, H_2\} \]
\[ C_7 = \{X_3, H_3\} \]
\[ C_8 = \{X_4, H_4\} \]
\[ C_9 = \{X_5, H_5\} \]
Example - HMM

\[ \psi_k = \Pr(H_{t+1} | H_t) \quad \psi_k = \Pr(X_t | H_t) \]
Queries

Inference

Marginal distribution

$$Pr(X_1, X_2|e)$$

Likelihood of evidence

$$l(\vec{X}[1], \ldots, \vec{X}[M]; \Psi) = \prod_{m=1}^{M} Pr(X[m]_1, \ldots, X[m]_n; \Psi)$$

Model estimation

Maximum Likelihood

$$\arg \max_\Psi \left(l(\vec{X}[1], \ldots, \vec{X}[M]; \Psi)\right)$$
Approximate Inference

Sampling methods

Gibbs sampling

Variational approaches

Mean Field Belief propagation
(Our) Motivation

Relational models for huge interaction networks

Picture adopted from Yu et al 2008
Relational Probabilistic Graphical Models

\[ Pr(X_1, \ldots, X_n) = \frac{1}{Z(\Psi)} \prod_{t=1}^{T} \prod_{i \in I(t)} \psi_t(C_i) \]

\[ \Psi = \{\psi_t\}_{t=1}^{T} : \]

The **template** parameterization

\[ I(t) : \]

The set of features mapped to the \( t \)'th parameter

Friedman et al. 1999, Getoor et al. 2001
HMM revisited

\[ \psi_1 = Pr(X_t|H_t) \quad \psi_2 = Pr(H_{t+1}|H_t) \]

\[ P(X_1, \ldots, X_5, H_1, \ldots, H_5) = \prod_{k=1}^{4} \Psi_1(C_k) \prod_{k=5}^{9} \Psi_2(C_k) \]
Library Design

• Efficiency
  • Programming language: C++
  • Representation
  • Repeated calculations

• Enable extensions
  • Simple, well documented base classes

• Usage
  • Command line
  • API
FastInf Features

• Inference
  • Belief propagation (BP)
    • Generalized BP (Yedidia et al. 2005)
    • Tree ReWeighted BP (Wainwright et al. 2005)
    • Convexified Bethe approximations (Meshi et al. 2009)
  • Mean Field
  • Gibbs sampling

• Parameter estimation
  • Conjugate gradient descent, EM

• Documentation (partial):
  • http://compbio.cs.huji.ac.il/FastInf
### Comparison

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Applications

• Protein-protein interactions networks  Jaimovich et al. 2006
• Design of new belief propagation schemes  Elidan et al. 2006
• Protein design  Fromer et al. 2008
• Cryo ET image alignment  Amat et al. 2008
• Object localization of cluttered images  Heitz et al. 2009
External Libraries

- Boost c++ libraries
- GNU Scientific Library (GSL)
- GNU Linear Programing Kit (GLPK)

Liscence

- GPLv3
Demo
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