Approximate Inference

Part 1 of 2

Tom Minka

Microsoft Research, Cambridge, UK

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http://mlg.eng.cam.ac.uk/mlss09/

Bayesian paradigm

- Consistent use of probability theory for representing unknowns (parameters, latent variables, missing data)

Model

Data

Posterior Distribution → Decisions

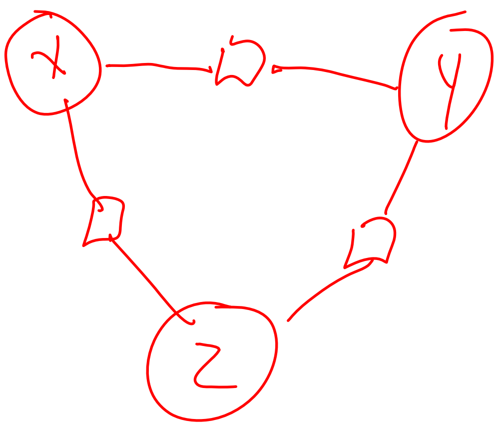
More Data

Bayesian paradigm

- Bayesian posterior distribution summarizes what we've learned from training data and prior knowledge
- Can use posterior to:
  - Describe training data
  - Make predictions on test data
  - Incorporate new data (online learning)
- Today's question: How to efficiently represent and compute posteriors?

Factor graphs

- Shows how a function of several variables can be factored into a product of simpler functions
- $f(x,y,z) = (x+y)(y+z)(x+z)$
- Very useful for representing posteriors

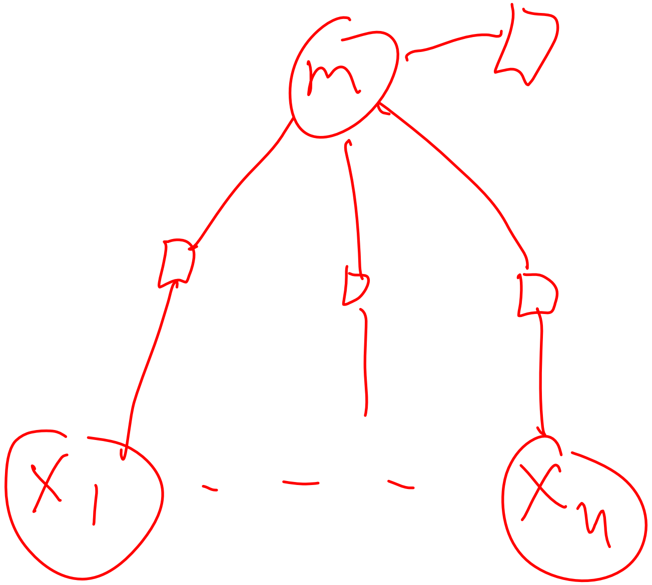


$$p(x) \prod_i p(y_i \mid x) = p(x, \vec{y})$$

Example factor graph

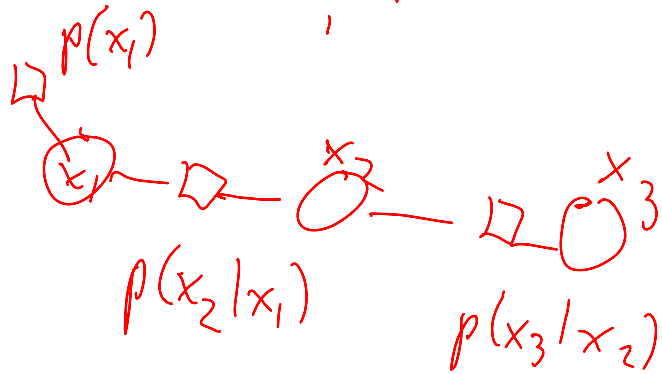
$$p(x_i \mid m) = N(x_i; m, 1)$$

$$p(m \mid x_1, \ldots, x_N) \propto p(m) \prod_i p(x_i \mid m)$$



$$p(x_1, \ldots, x_n)$$

$$= p(x_1) \prod_i p(x_i \mid x_{i-1})$$



Two tasks

- Modeling
  - What graph should I use for this data?
- Inference
  - Given the graph and data, what is the mean of x (for example)?
  - Algorithms:
    - Sampling
    - Variable elimination
    - Message-passing (Expectation Propagation, Variational Bayes, …)

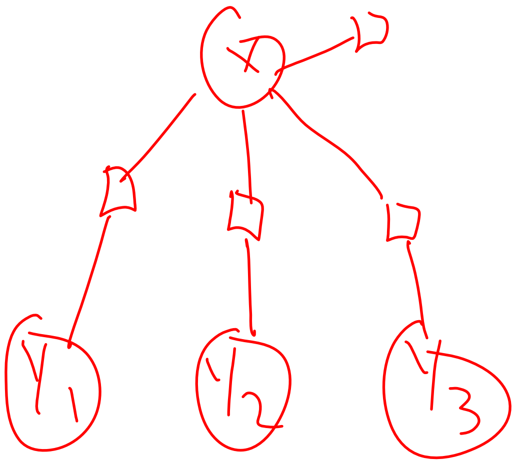
A (seemingly) intractable problem

Clutter problem

- Want to estimate x given multiple y's

$$p(x) = \mathcal{N}(x; 0, 100)$$

$$p(y_i|x) = (0.5)\mathcal{N}(y_i; x, 1) + (0.5)\mathcal{N}(y_i; 0, 10)$$

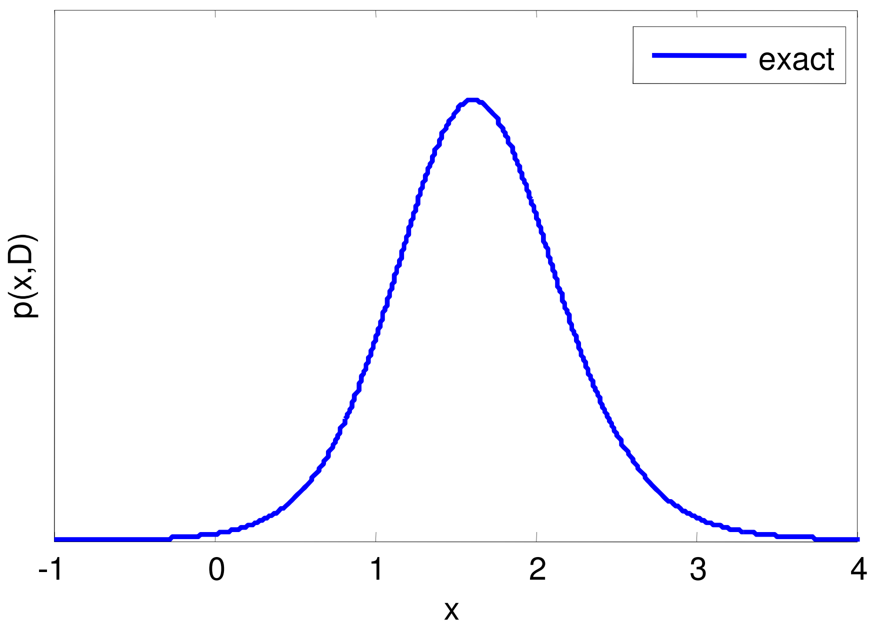


$\underline{p(x|y_1, \dots, y_n)} \propto p(x) \prod_i p(y_i|x)$

$\underline{p(x)p(y_1|x)p(y_2|x)}$

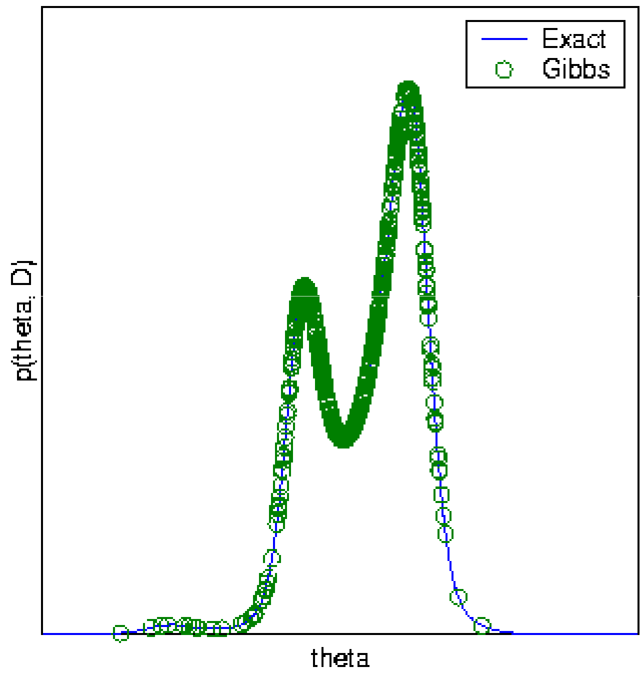
2 pts -> 4 Gs   n pts -> 2^n

Exact posterior



Representing posterior distributions

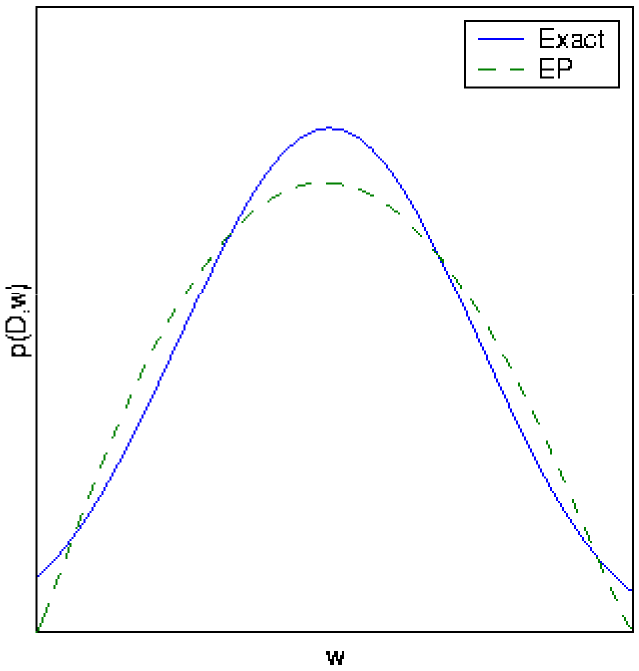
Sampling



Good for complex,
multi-modal distributions

Slow, but predictable accuracy

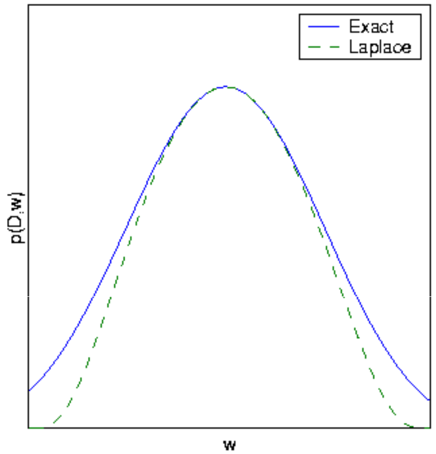
Deterministic approximation



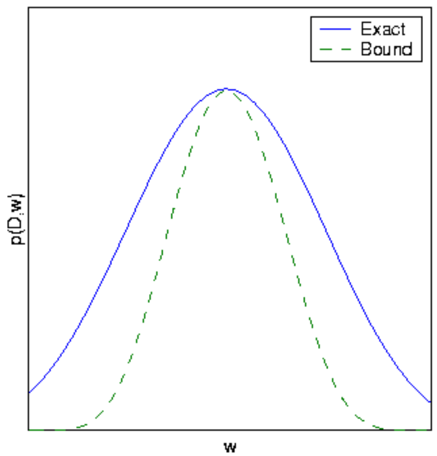
Good for simple,
smooth distributions

Fast, but unpredictable accuracy

Deterministic approximation

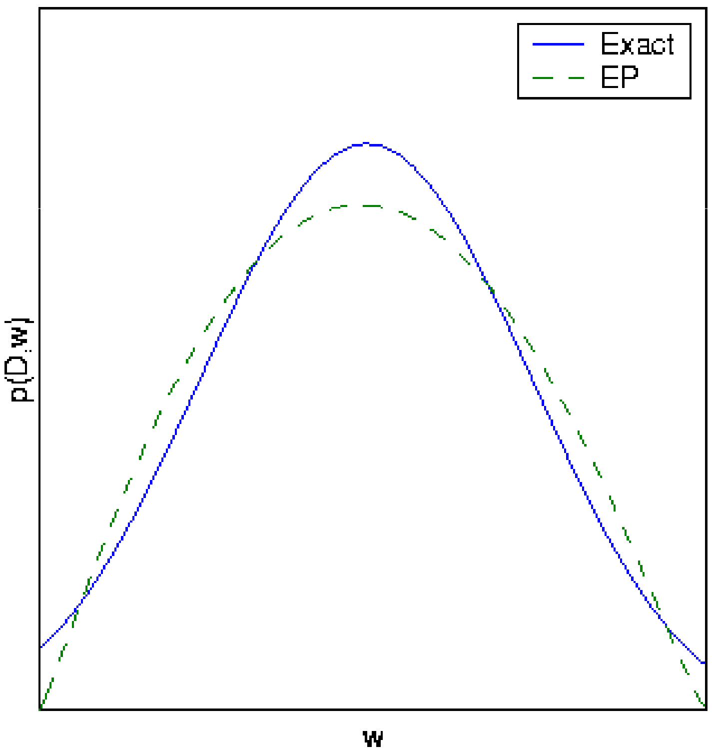


Laplace's method
• Bayesian curve fitting, neural networks (MacKay)
• Bayesian PCA (Minka)



Variational bounds
• Bayesian mixture of experts (Waterhouse)
• Mixtures of PCA (Tipping, Bishop)
• Factorial/coupled Markov models (Ghahramani, Jordan, Williams)

Moment matching



Another way to perform deterministic approximation

• Much higher accuracy on some problems

Assumed-density filtering (1984)

Loopy belief propagation (1997)

Expectation Propagation (2001)

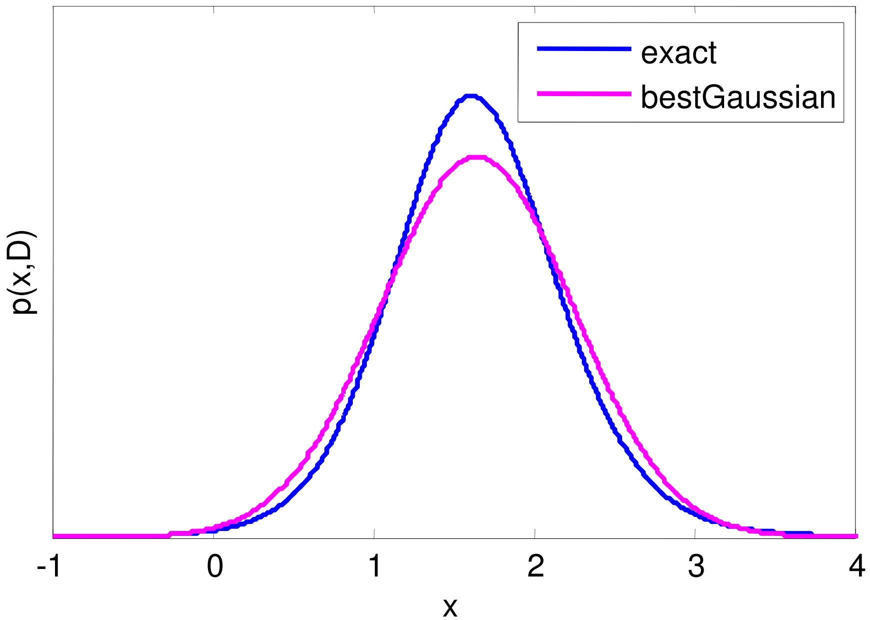
Today

- Moment matching
  (Expectation Propagation)

Tomorrow

- Variational bounds
  (Variational Message Passing)

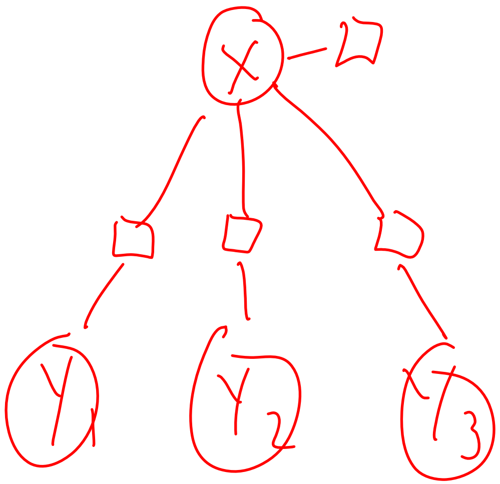
Best Gaussian by moment matching

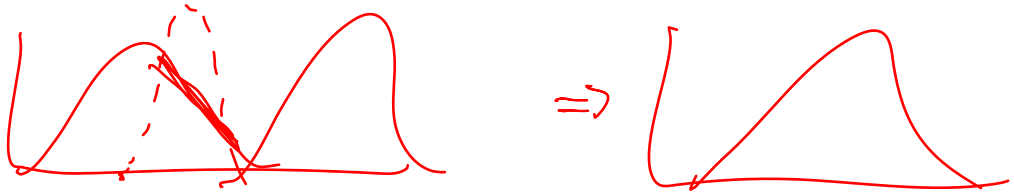


Strategy

- Approximate *each* factor by a Gaussian in x

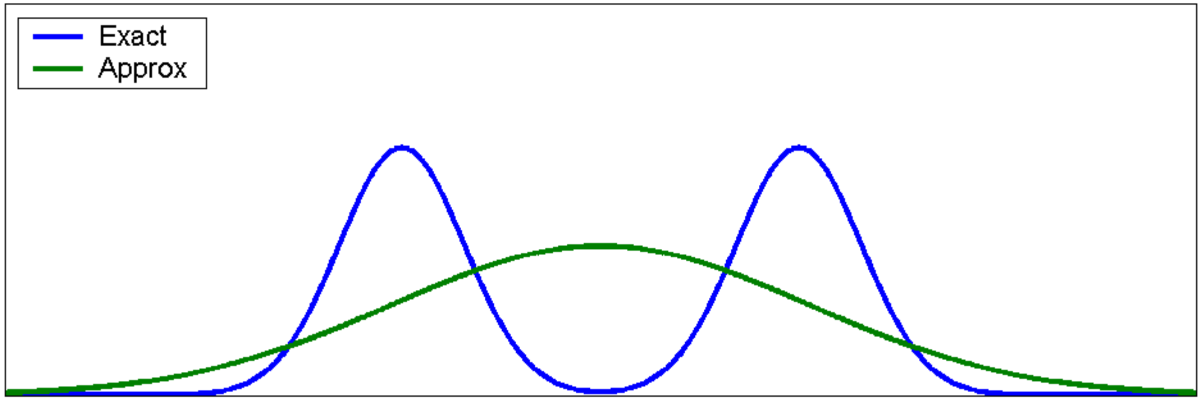
$$
\begin{aligned}
p(y_i|x) &= (0.5)\mathcal{N}(y_i; x, 1) + (0.5)\mathcal{N}(y_i; 0, 10) \\
&\approx \mathcal{N}(x; m_i, v_i)
\end{aligned}
$$





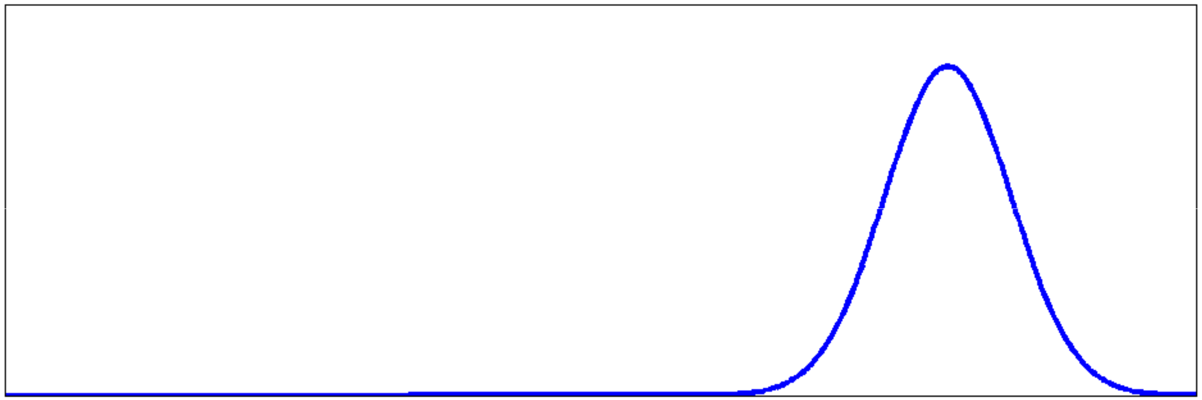
Approximating a single factor

(naïve)



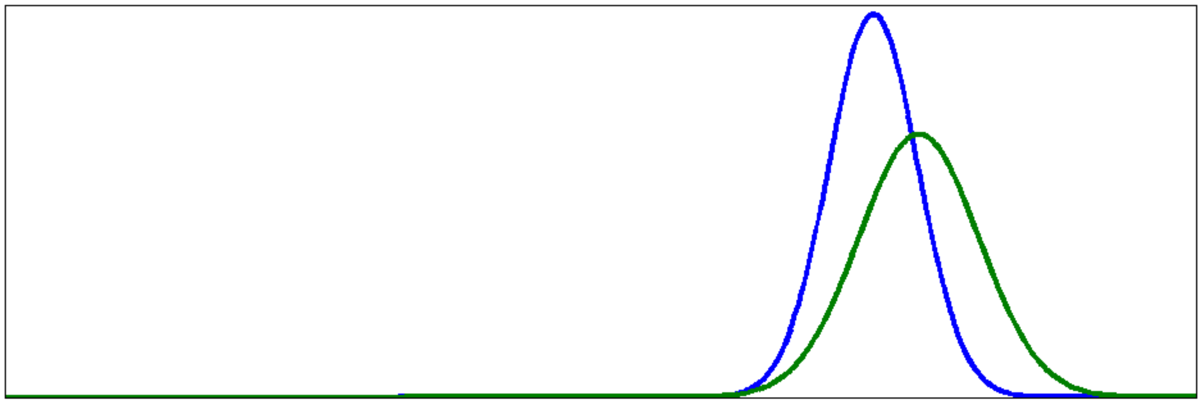
$f_i(x)$

$\times$



$q^{\backslash i}(x)$

$=$



$p(x)$

(informed)

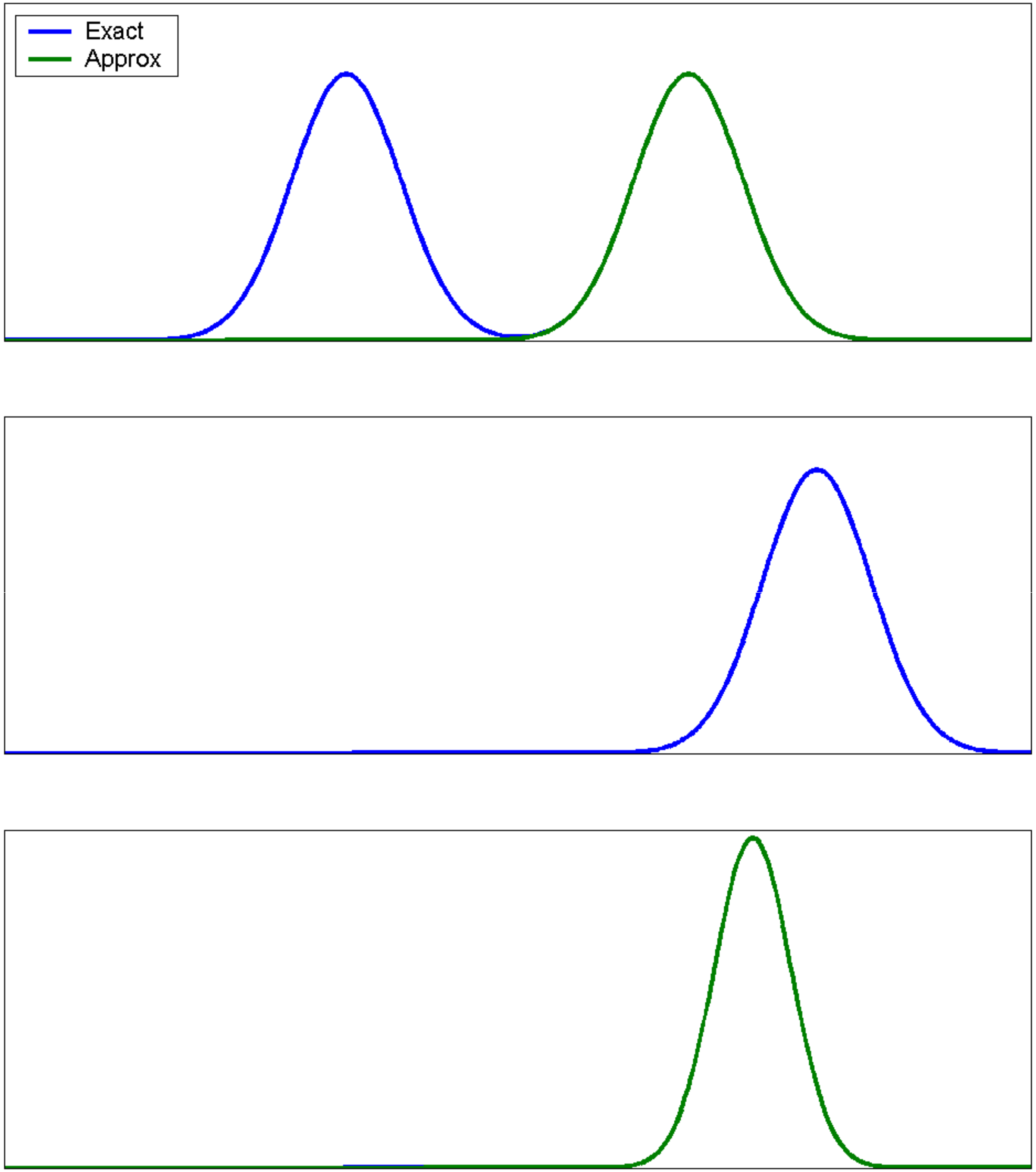
$f_i(x)$

$\times$

$q^{\backslash i}(x)$

$=$

$p(x)$

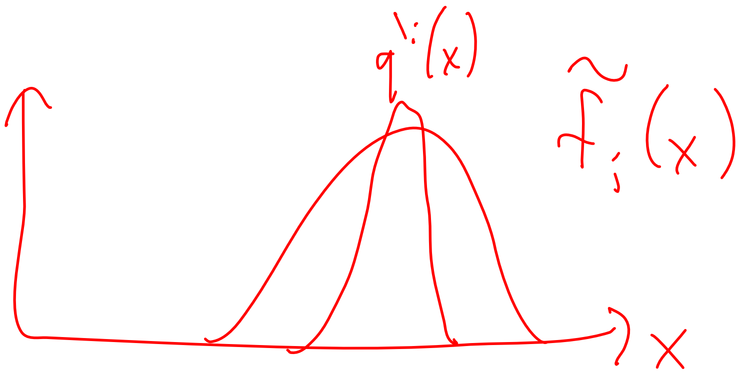


Single factor with Gaussian context

f_i = anything $\quad q^{\setminus i}$ = Gaussian

$\tilde{f}_i$ = Gaussian

$$f_i(x)\, q^{\setminus i}(x) \approx \tilde{f}_i(x)\, q^{\setminus i}(x)$$



$$\mathrm{proj}\left[f_i(x)\, q^{\setminus i}(x)\right] = \tilde{f}_i(x)\, q^{\setminus i}(x)$$

$$\tilde{f}_i(x) = \frac{\mathrm{proj}\left[f_i(x)\, q^{\setminus i}(x)\right]}{q^{\setminus i}(x)}$$

$$\mathrm{proj}\left[p(x)\right] = \tilde{p}(x)$$

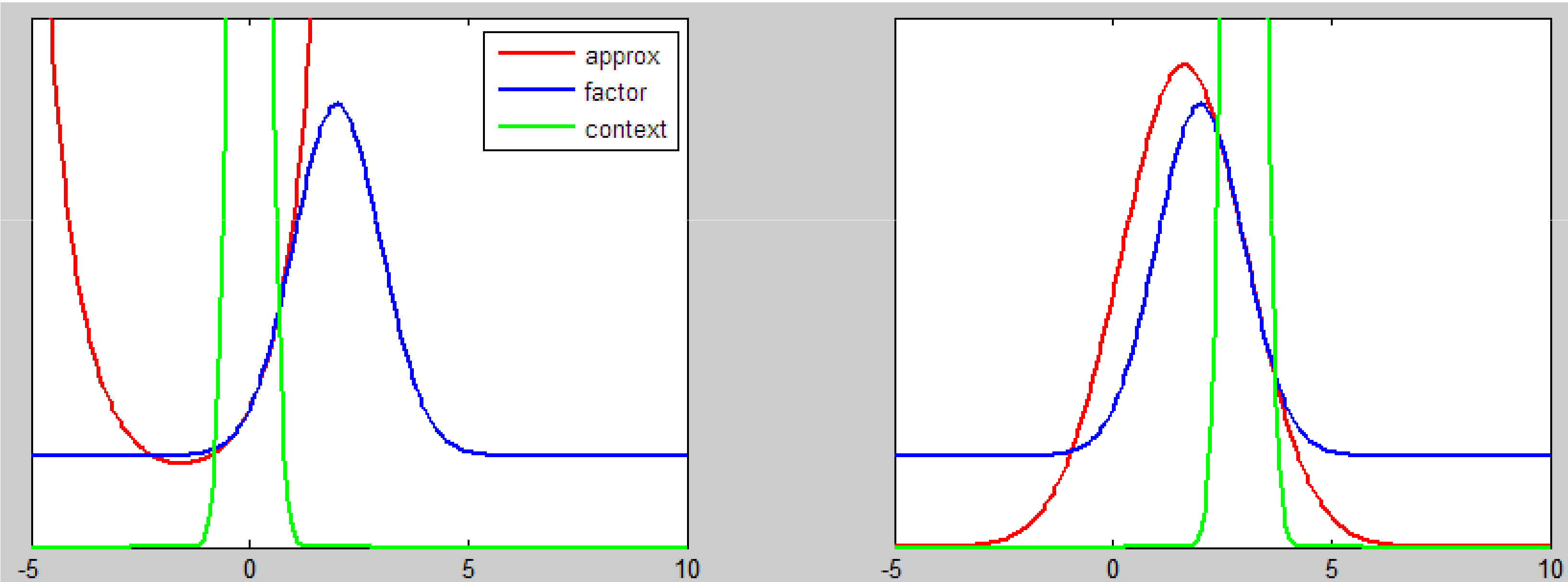
same moments

Gaussian multiplication formula

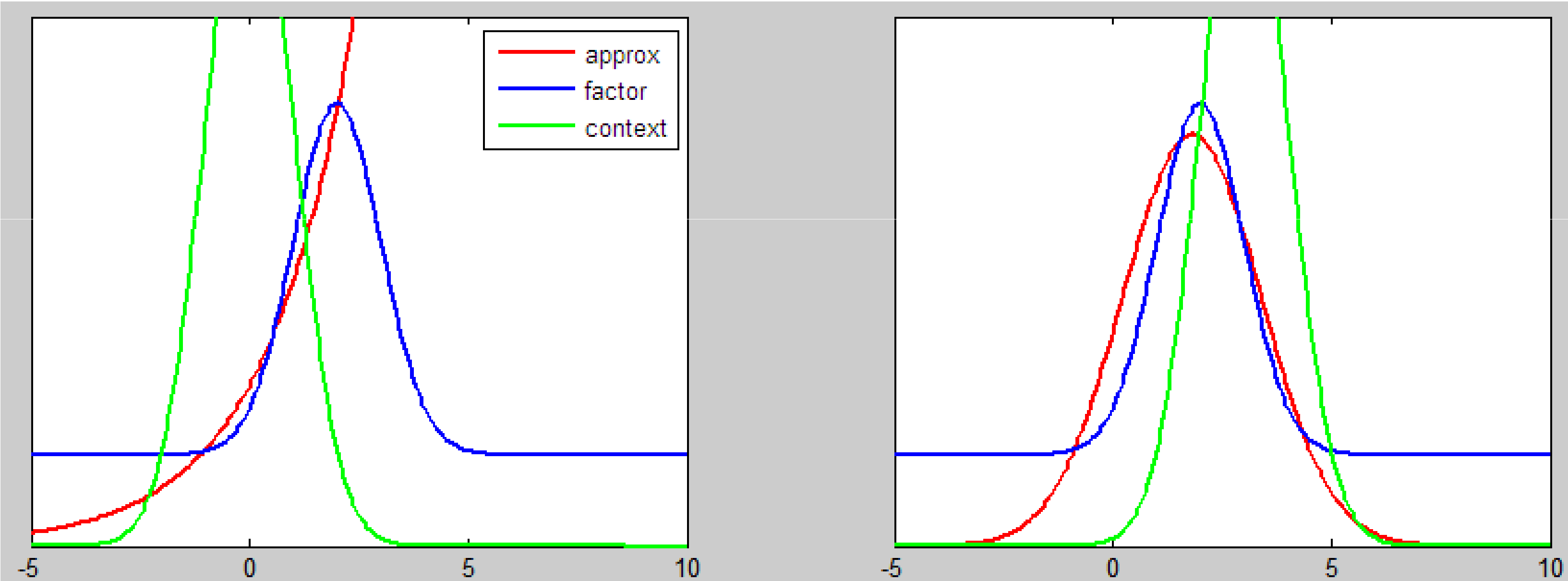
$$
\begin{aligned}
\mathcal{N}(x; m_1, v_1)\mathcal{N}(x; m_2, v_2) &= \mathcal{N}(m_1; m_2, v_1 + v_2)\mathcal{N}(x; m, v) \\
\text{where } v &= \frac{1}{\frac{1}{v_1} + \frac{1}{v_2}} \\
m &= v\left(\frac{m_1}{v_1} + \frac{m_2}{v_2}\right)
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{N}(x; m_1, v_1)/\mathcal{N}(x; m_2, v_2) &= \frac{v_2 \mathcal{N}(x; m, v)}{(v_2 - v_1)\mathcal{N}(m_1; m_2, v_2 - v_1)} \\
\text{where } v &= \frac{1}{\frac{1}{v_1} - \frac{1}{v_2}} \\
m &= v\left(\frac{m_1}{v_1} - \frac{m_2}{v_2}\right)
\end{aligned}
$$

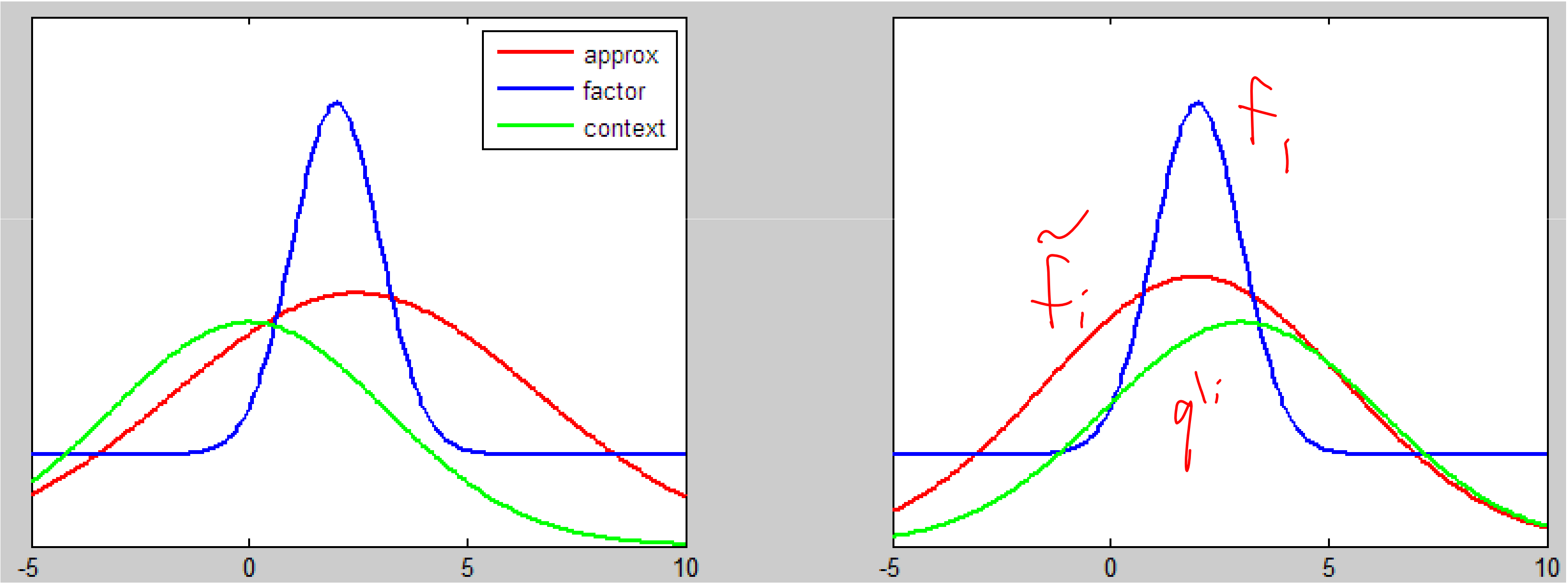
Approximation with narrow context



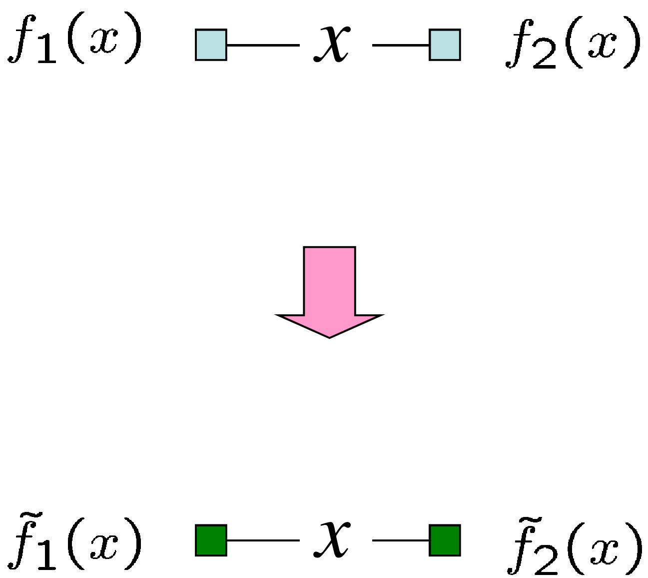
Approximation with medium context



Approximation with wide context



Two factors



$\tilde f_1(x)\tilde f_2(x) = \text{proj}[f_1(x)\tilde f_2(x)]$

$$\tilde{f}_1(x) = \frac{\text{proj}[f_1(x)\tilde{f}_2(x)]}{\tilde{f}_2(x)}$$

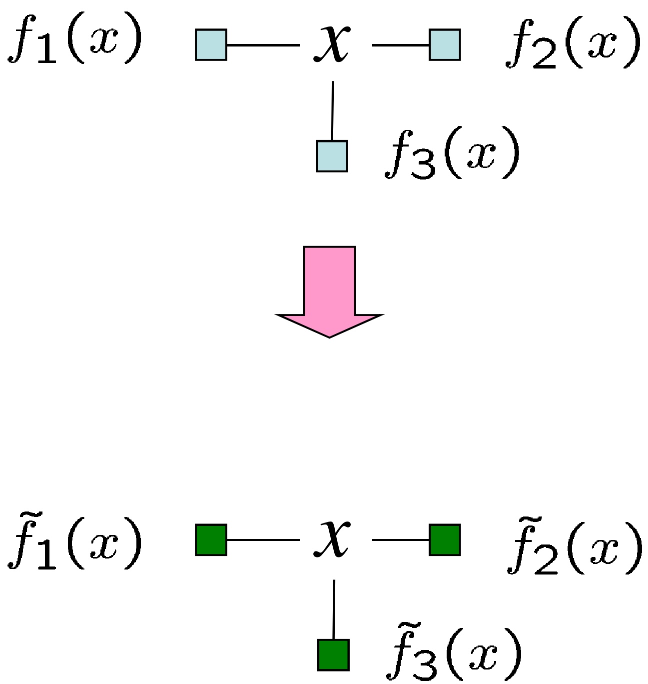
$$\tilde{f}_2(x) = \frac{\text{proj}[f_2(x)\tilde{f}_1(x)]}{\tilde{f}_1(x)}$$

$\tilde f_1(x)\tilde f_2(x) = \text{proj}[f_2(x)\tilde f_1(x)]$

Message passing

$\text{proj}[f_1(x)f_2(x)] \neq \tilde f_1 \tilde f_2$

Three factors



$$\tilde{f}_1(x) = \frac{\mathrm{proj}\left[f_1(x)\,\tilde{f}_2(x)\,\tilde{f}_3(x)\right]}{\tilde{f}_2(x)\,\tilde{f}_3(x)}$$

$$\tilde{f}_2(x) = \frac{\mathrm{proj}\left[f_2(x)\,\tilde{f}_1(x)\,\tilde{f}_3(x)\right]}{\tilde{f}_1(x)\,\tilde{f}_3(x)}$$

Message passing

Message Passing = Distributed Optimization

$p(x) = \prod_i f_i(x)$ $\quad q(x) = \prod_i \tilde{f}_i(x)$

- Messages represent a simpler distribution $q(x)$ that approximates $p(x)$
  - A *distributed* representation
- Message passing = optimizing q to fit p
  - q stands in for p when answering queries
- Choices:
  - What type of distribution to construct (approximating family)
  - What cost to minimize (divergence measure)

Distributed divergence minimization

- Write p as product of factors:

$$p(x) = \prod_a f_a(x)$$

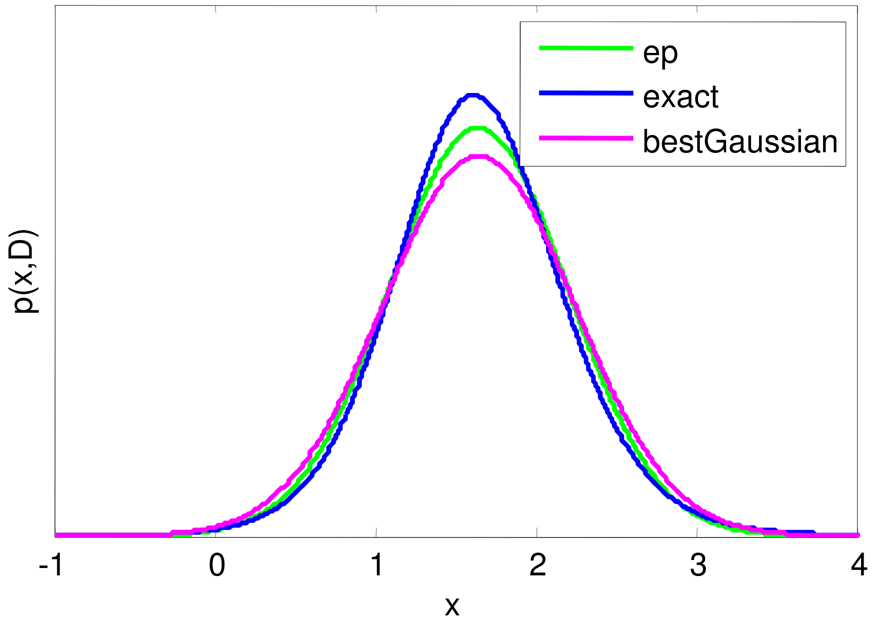
- Approximate factors one by one:

$$f_a(x) \rightarrow \tilde{f}_a(x)$$

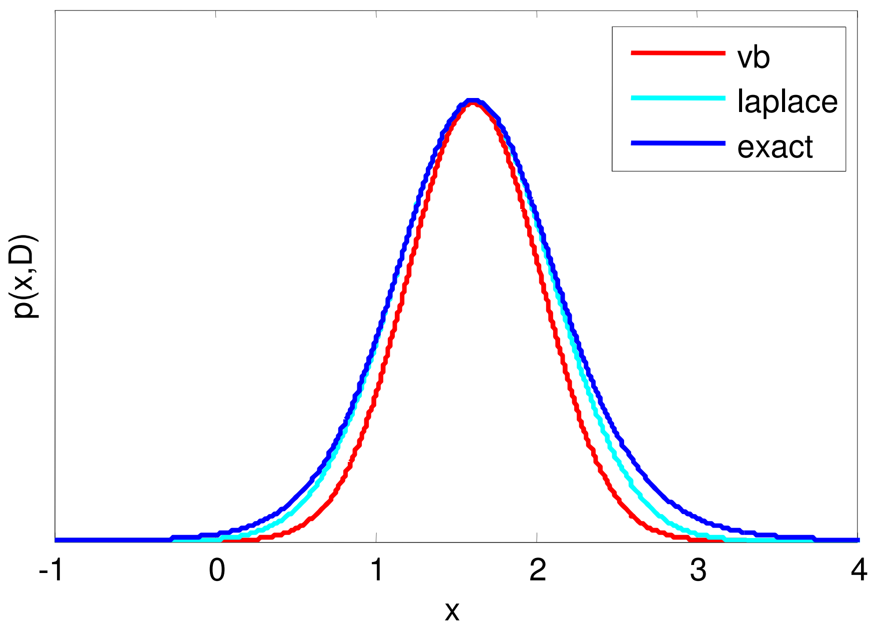
- Multiply to get the approximation:

$$q(x) = \prod_a \tilde{f}_a(x)$$

Gaussian found by EP



Other methods



Accuracy

Posterior mean:

exact = 1.64864

ep = 1.64514

laplace = 1.61946

vb = 1.61834

Posterior variance:

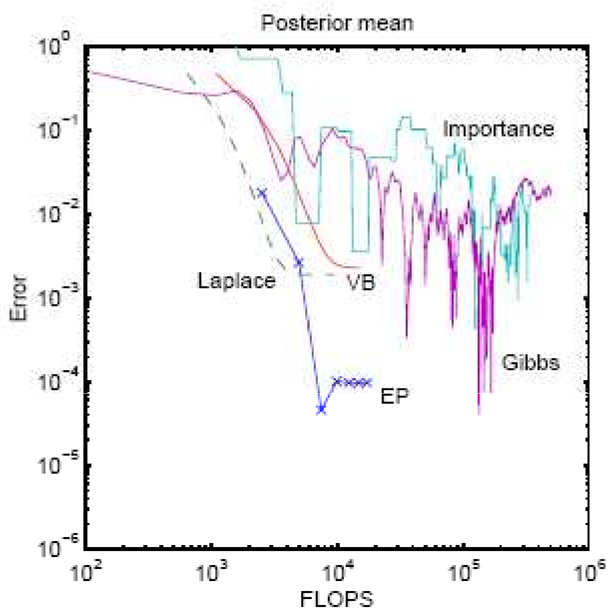
exact = 0.359673

ep = 0.311474

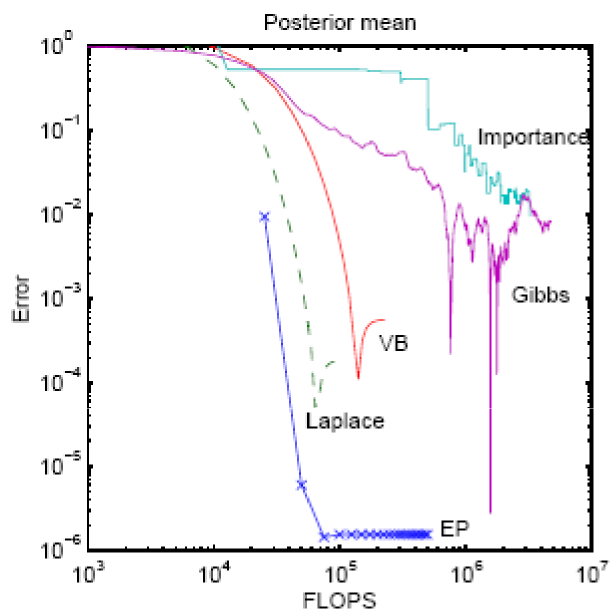
laplace = 0.234616

vb = 0.171155

Cost vs. accuracy



20 points



200 points

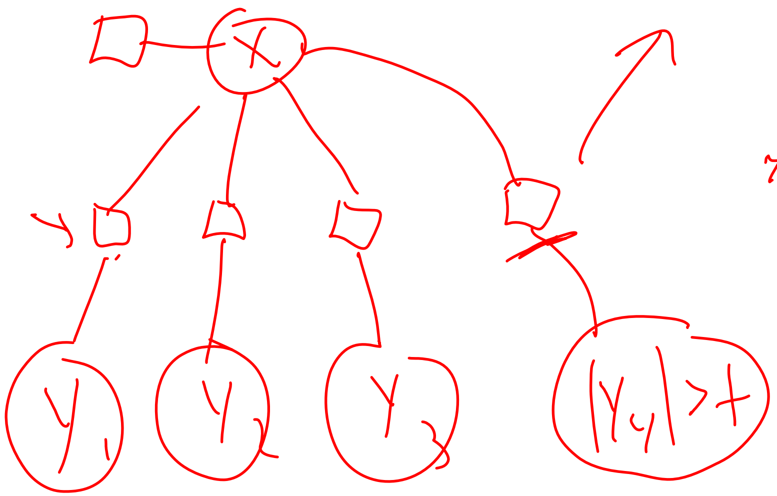
Deterministic methods improve with more data (posterior is more Gaussian)
Sampling methods do not

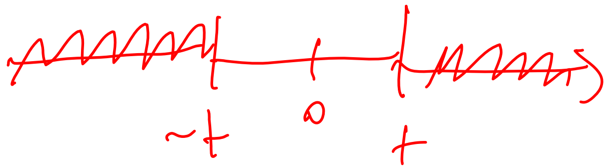
Censoring example

- Want to estimate x given multiple y's

$$p(x) = N(x;0,100) \qquad p(y_i \mid x) = N(y;x,1)$$

$$p(|y_i| > t \mid x) = \int_{-\infty}^{-t} N(y;x,1)\,dy + \int_{t}^{\infty} N(y;x,1)\,dy$$



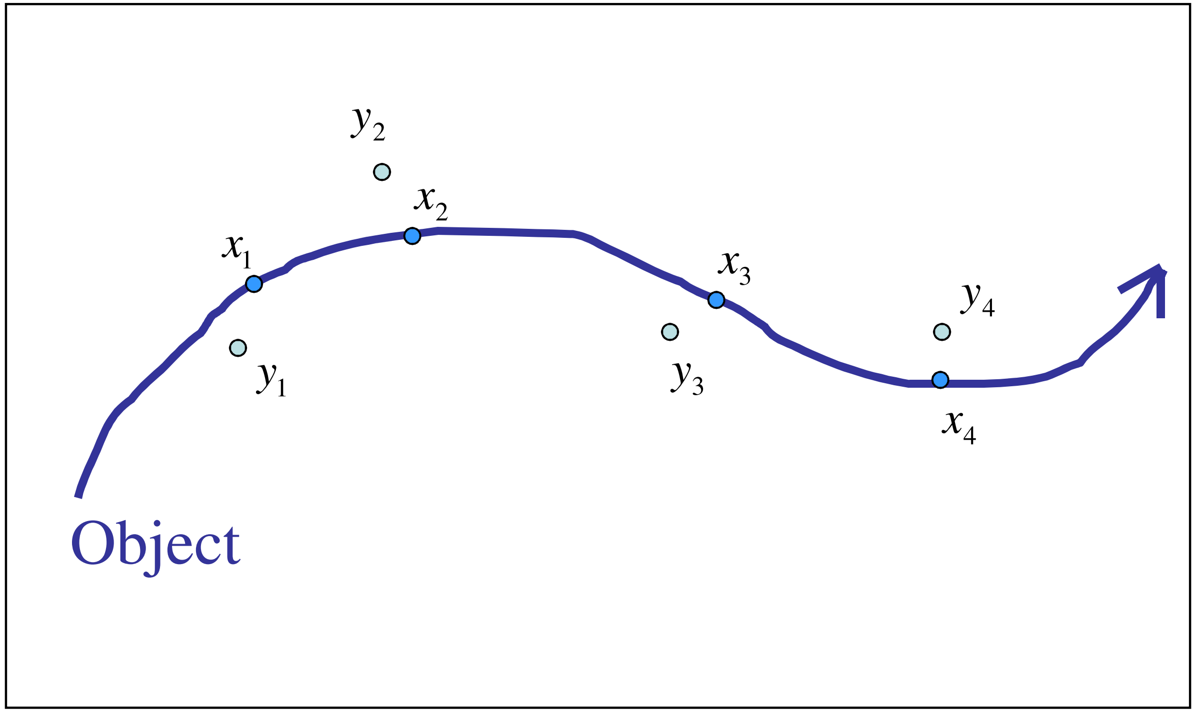


$$\frac{\mathrm{proj}\left[p(|y_i| > t \mid x)\, q^{\setminus i}(x)\right]}{q^{\setminus i}(x)} = \tilde{f}(x)$$

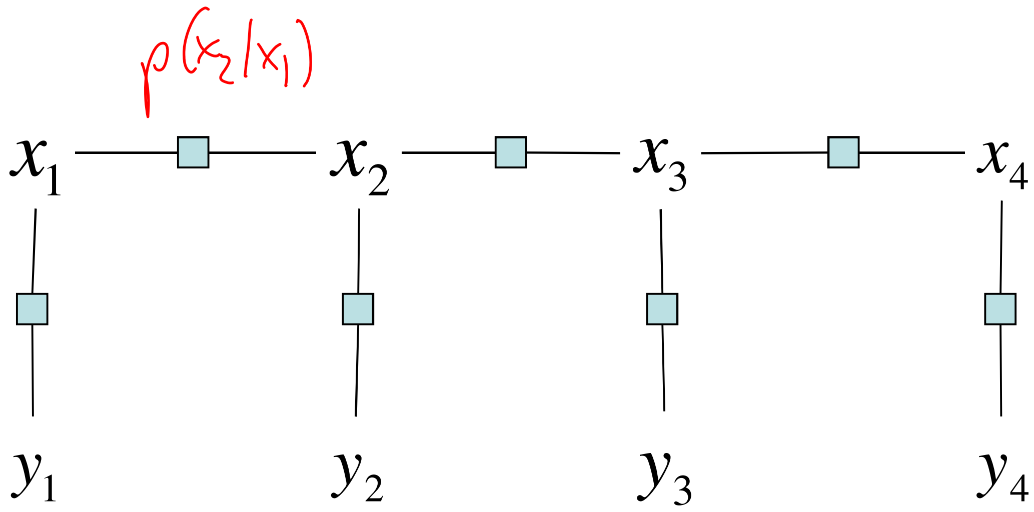
Time series problems

Example: Tracking

Guess the position of an object given noisy measurements



Factor graph

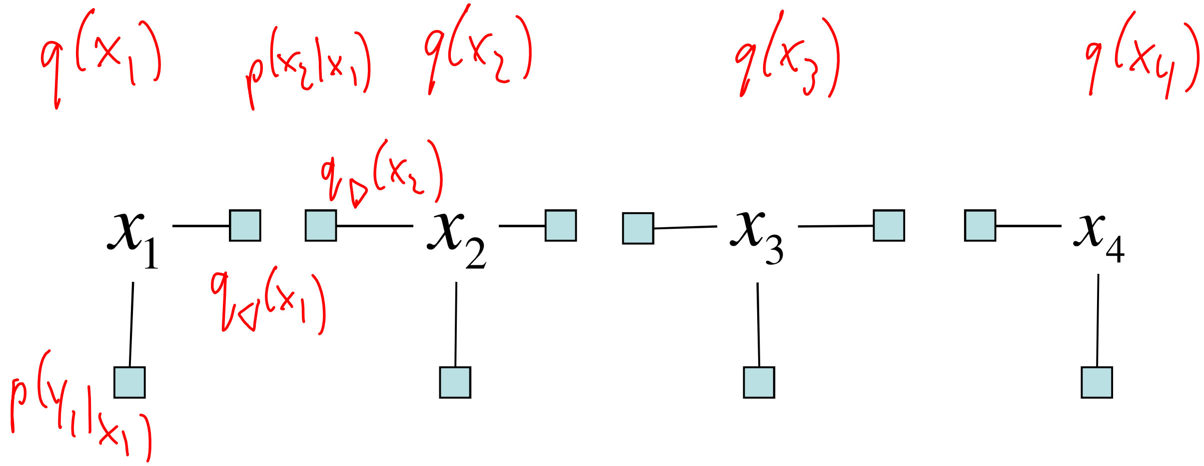


e.g. $x_t = x_{t-1} + v_t$ (random walk)

$$y_t = x_t + \text{noise}$$

want distribution of x's given y's

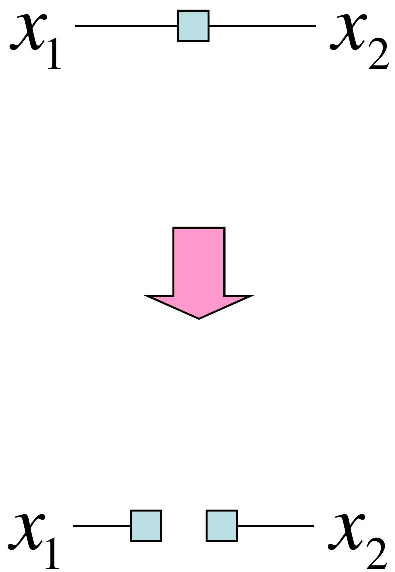
Approximate factor graph



$$p(x_2|x_1) \approx q_{\triangleleft}(x_1)\, q_{\triangleright}(x_2)$$

Splitting a pairwise factor

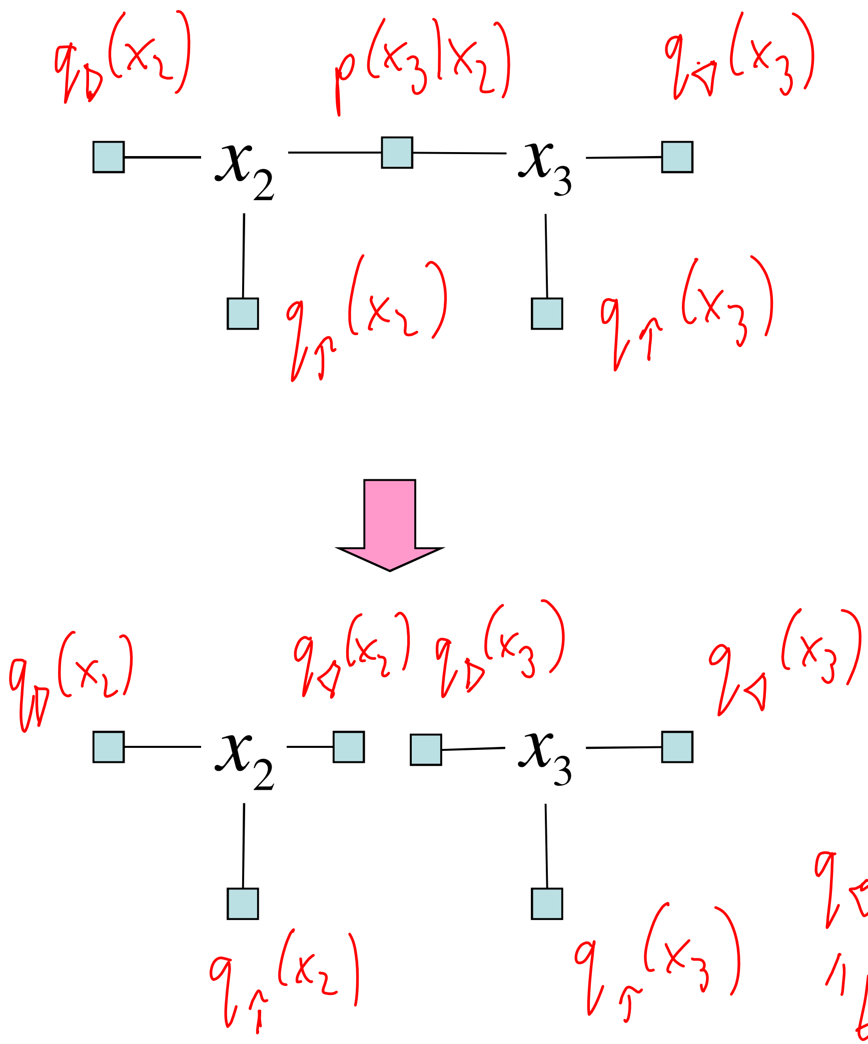
$p(x_2|x_1)$



$q_{\triangleleft}(x_1)\quad q_{\triangleright}(x_2)$

$$q_{\triangleleft}(x_1)\, q_{\triangleright}(x_2) = \underline{\text{proj}}\left[\, p(x_2|x_1) \,\right]$$

Splitting in context



$$q_\triangleright(x_2)\, q_\uparrow(x_2) \int p(x_3|x_2)\, q_\triangleleft(x_3)\, q_\uparrow(x_3)\, dx_3$$

$$\approx q_\triangleright(x_2)\, q_\uparrow(x_2)\, \underline{q_\triangleleft(x_2)}$$

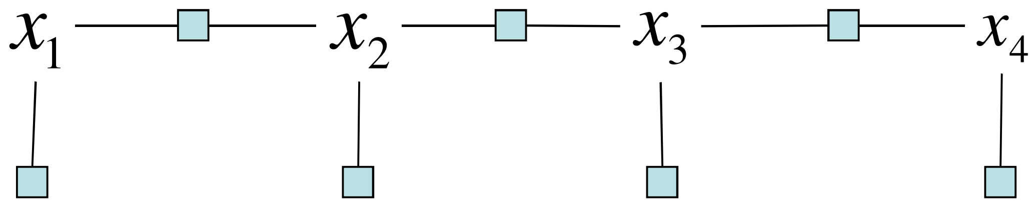
$$q_\triangleleft(x_2) = \text{proj}\left[q_\triangleright(x_2)\, q_\uparrow(x_2) \int \sim \right]$$

$$q_\triangleright(x_2)\, q_\uparrow(x_2)$$

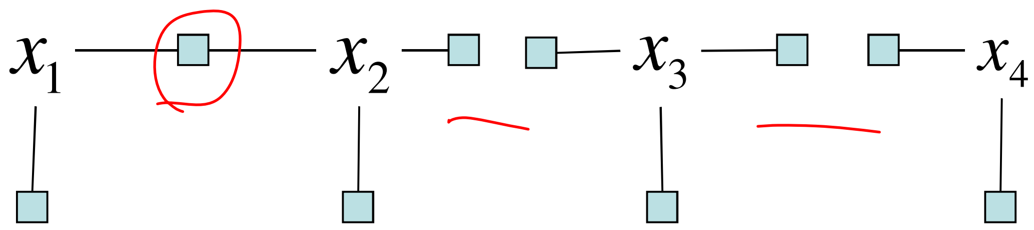
$$q_\triangleleft(x_2) = \int p(x_3|x_2)\, q_\triangleleft(x_3)\, q_\uparrow(x_3)\, dx_3$$

"backward message"

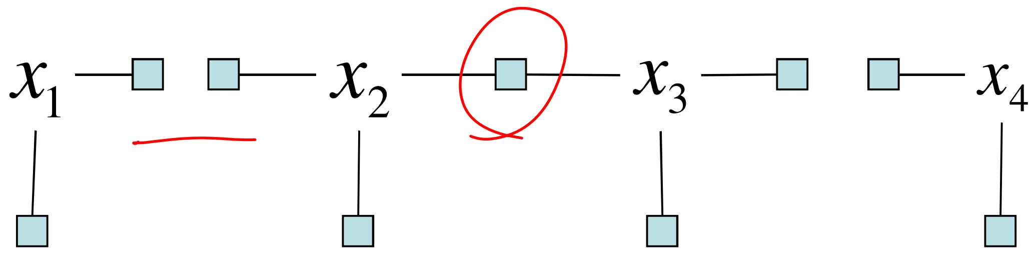
Sweeping through the graph



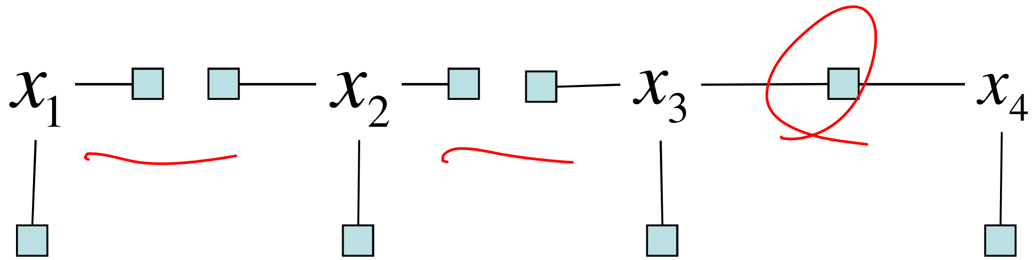
Sweeping through the graph



Sweeping through the graph

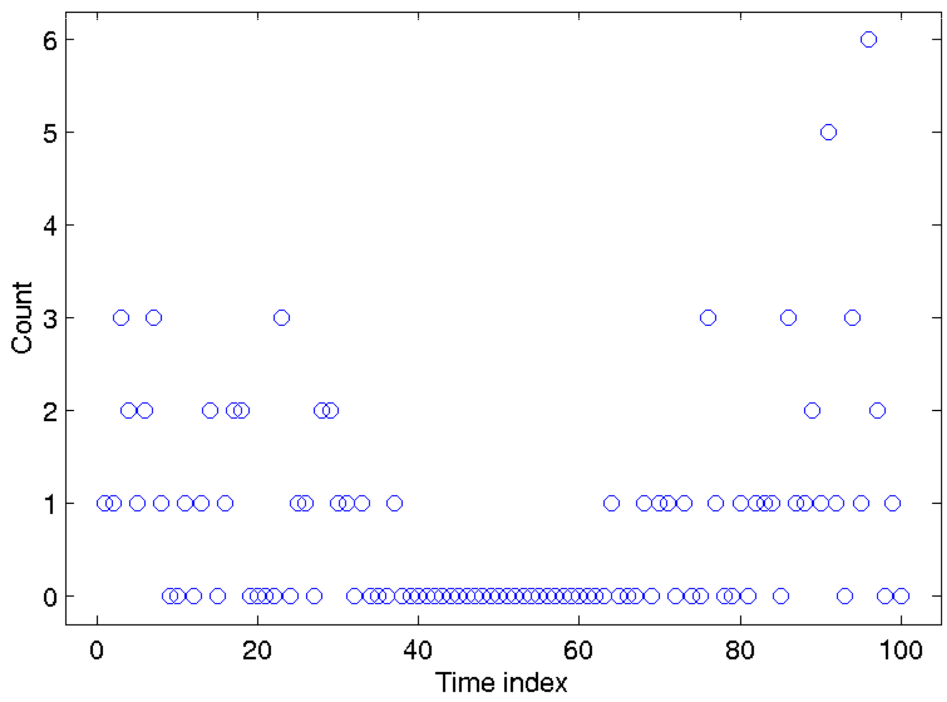


Sweeping through the graph



Example: Poisson tracking

- y_t is a Poisson-distributed integer with mean $\exp(x_t)$



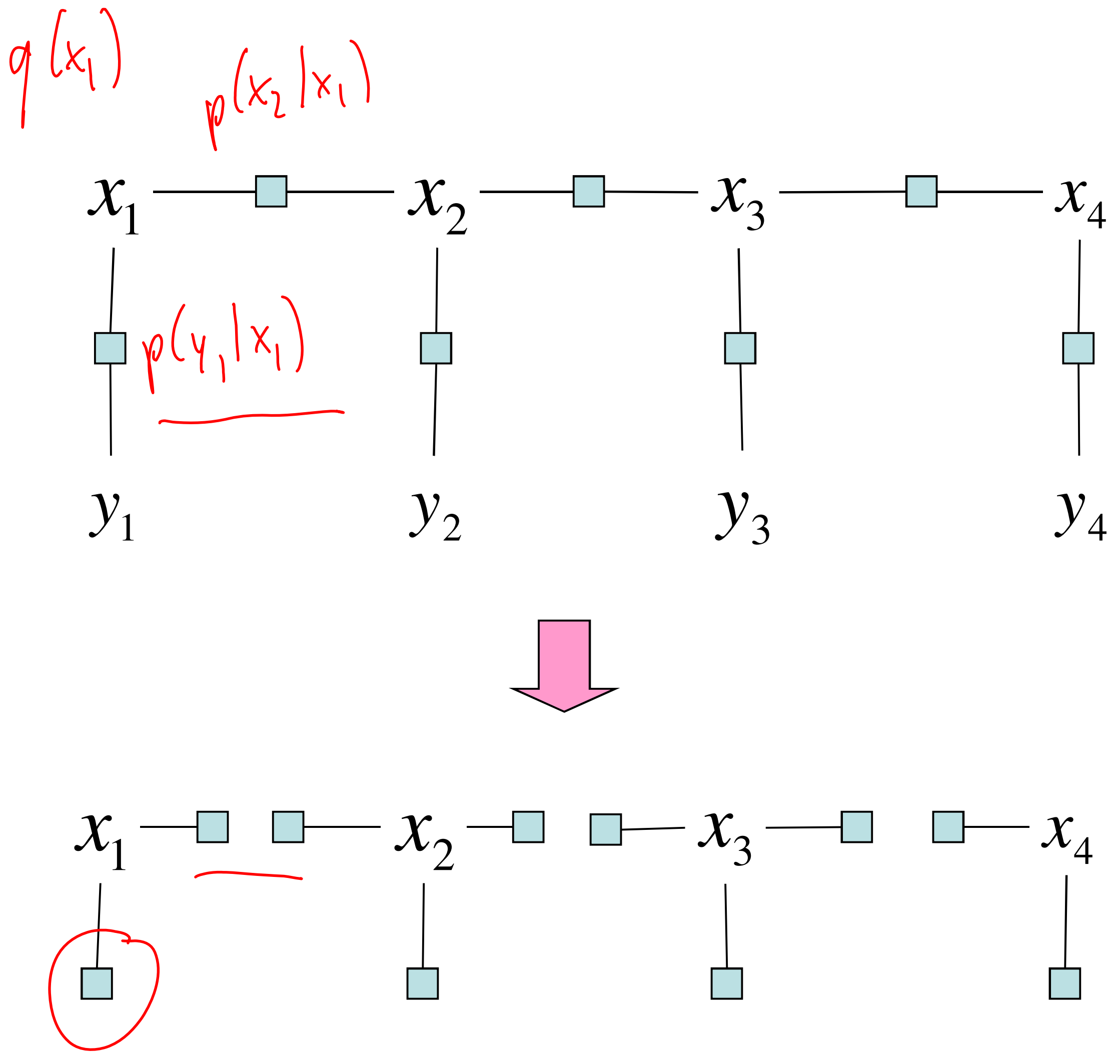
Poisson tracking model

$$p(x_1) \sim N(0,100)$$

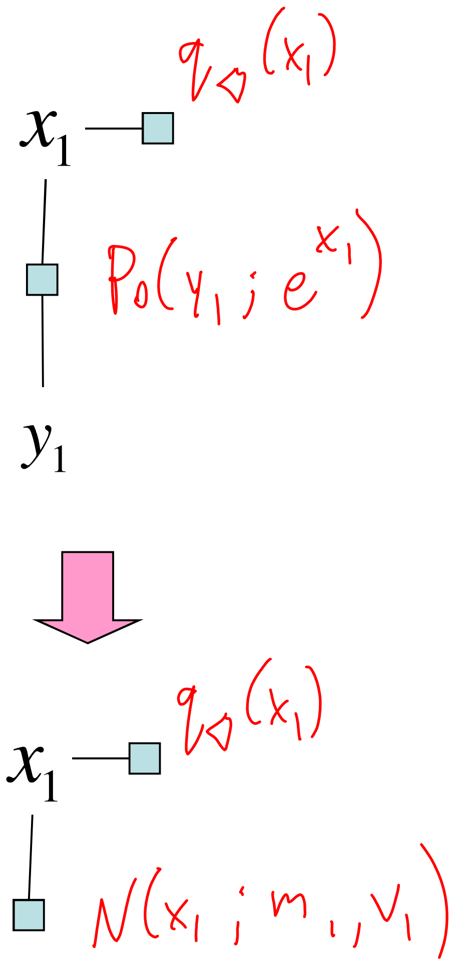
$$p(x_t \mid x_{t-1}) \sim N(x_{t-1}, 0.01)$$

$$p(y_t \mid x_t) = \exp(y_t x_t - e^{x_t}) / y_t!$$

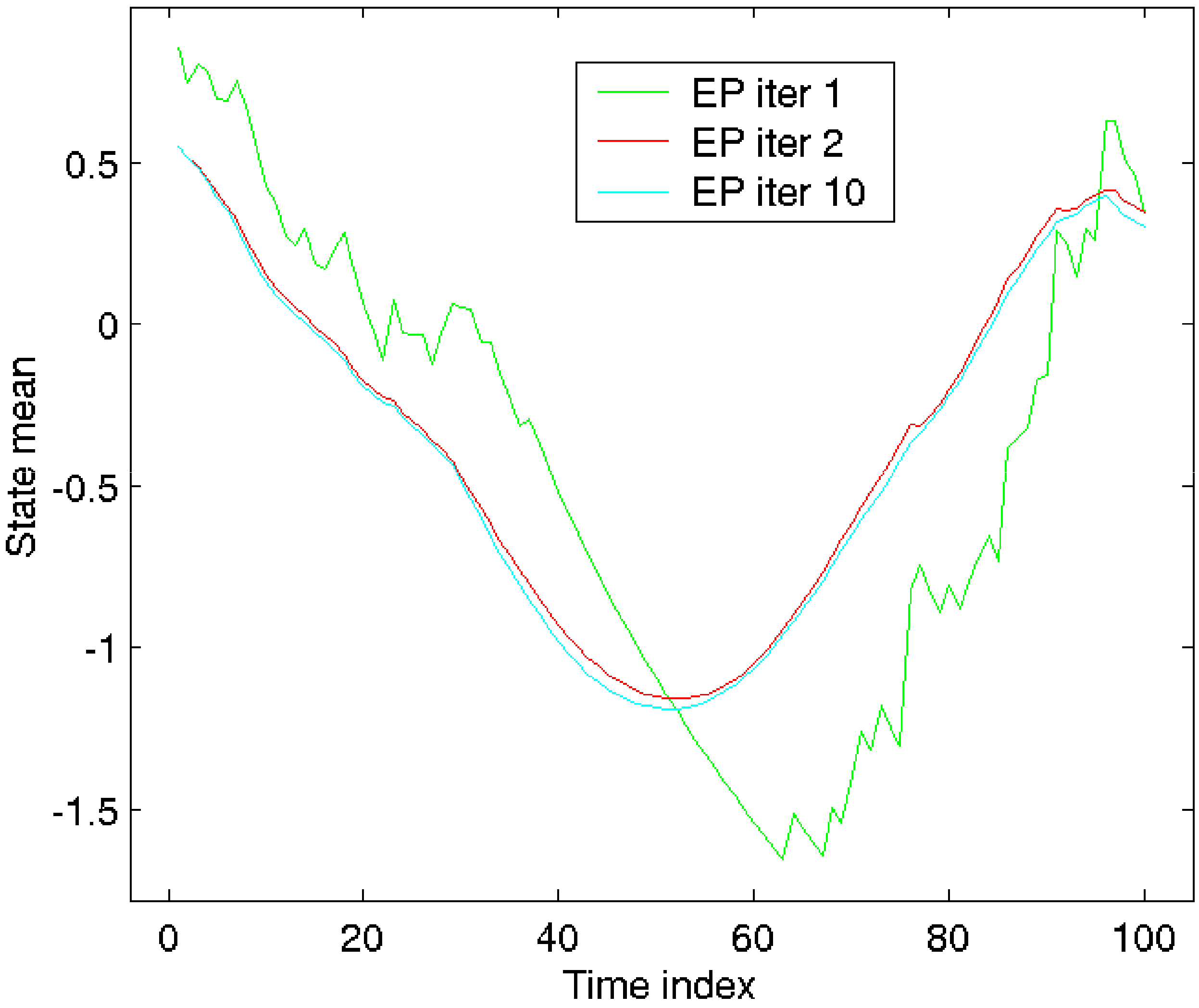
Factor graph



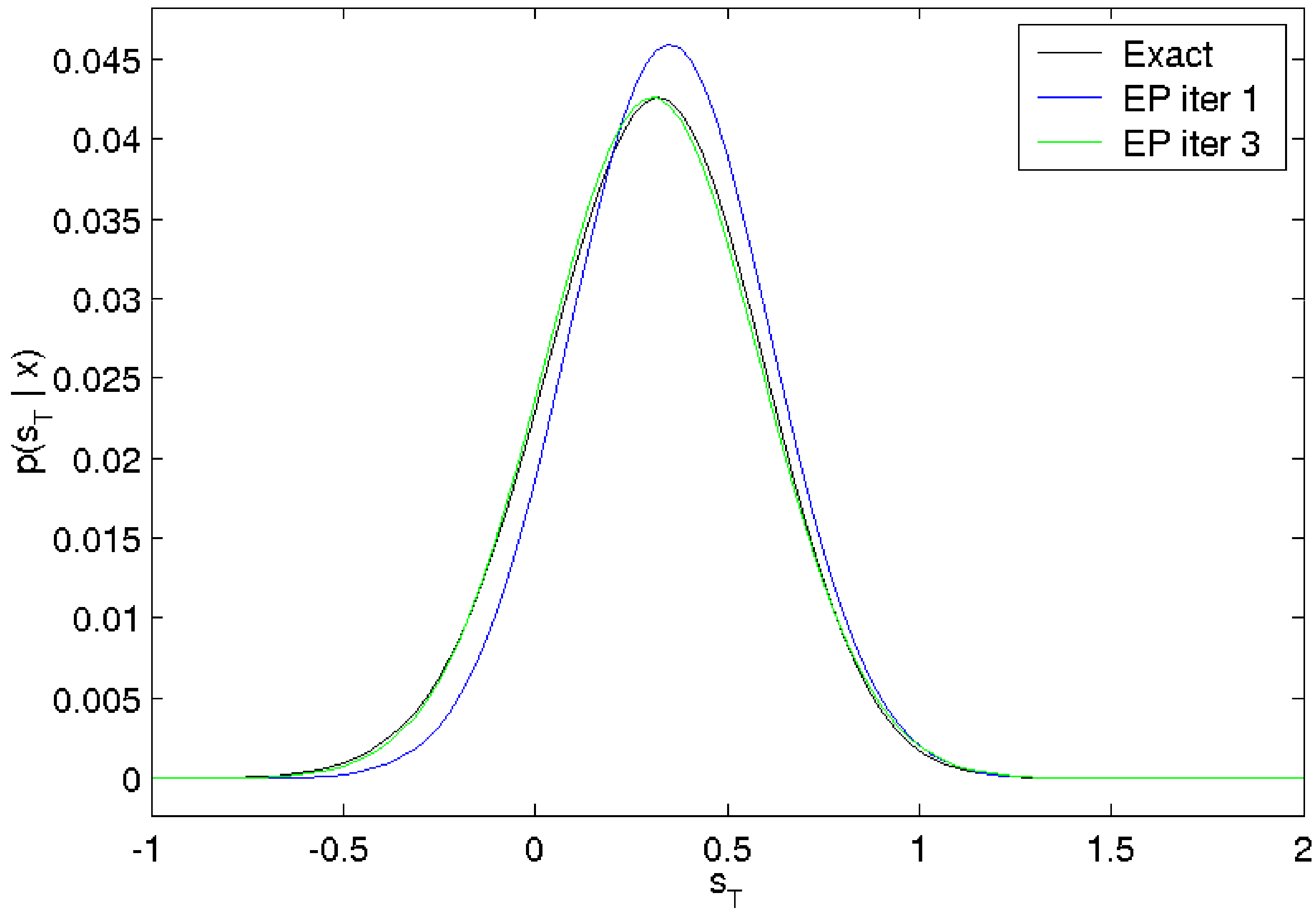
Approximating a measurement factor

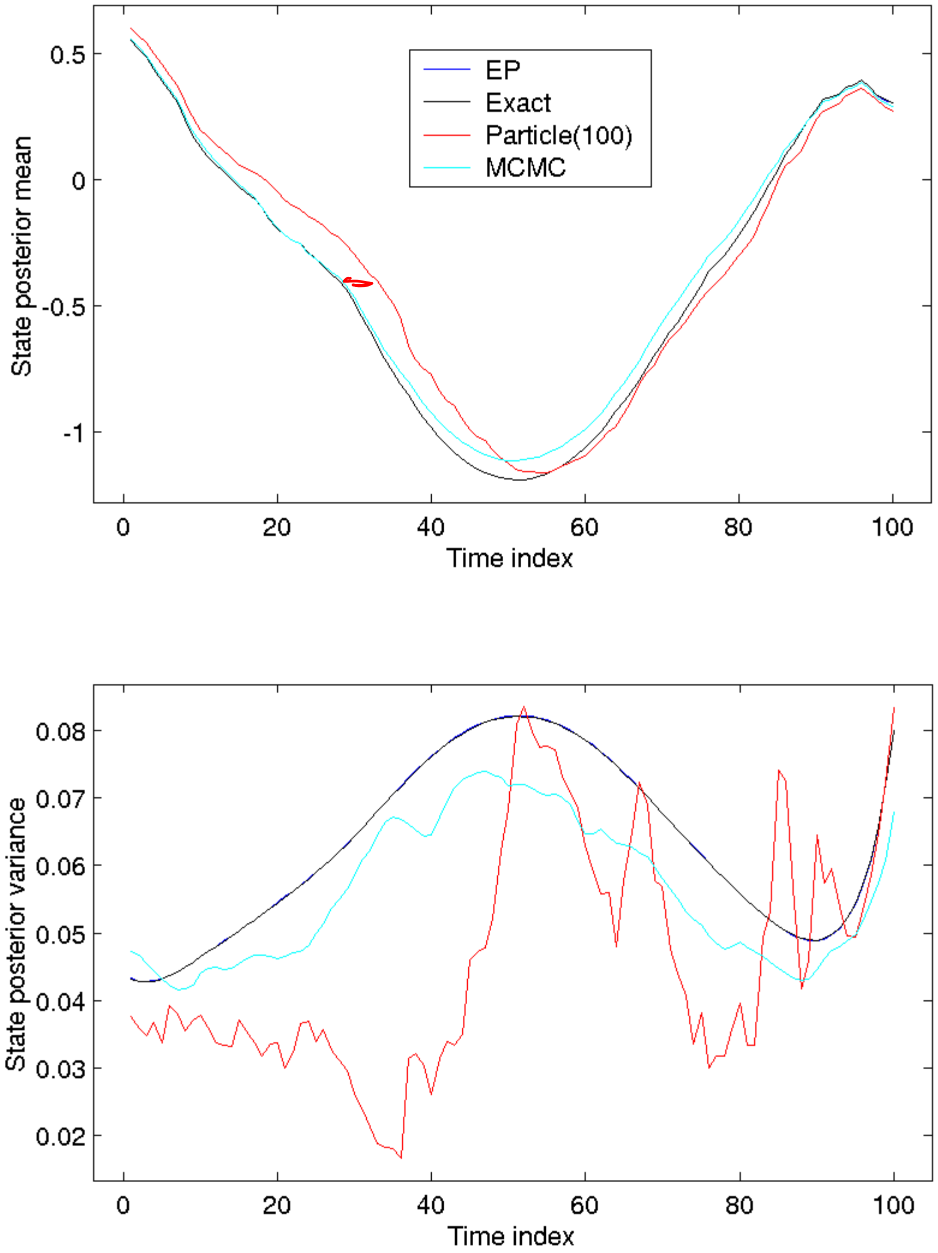


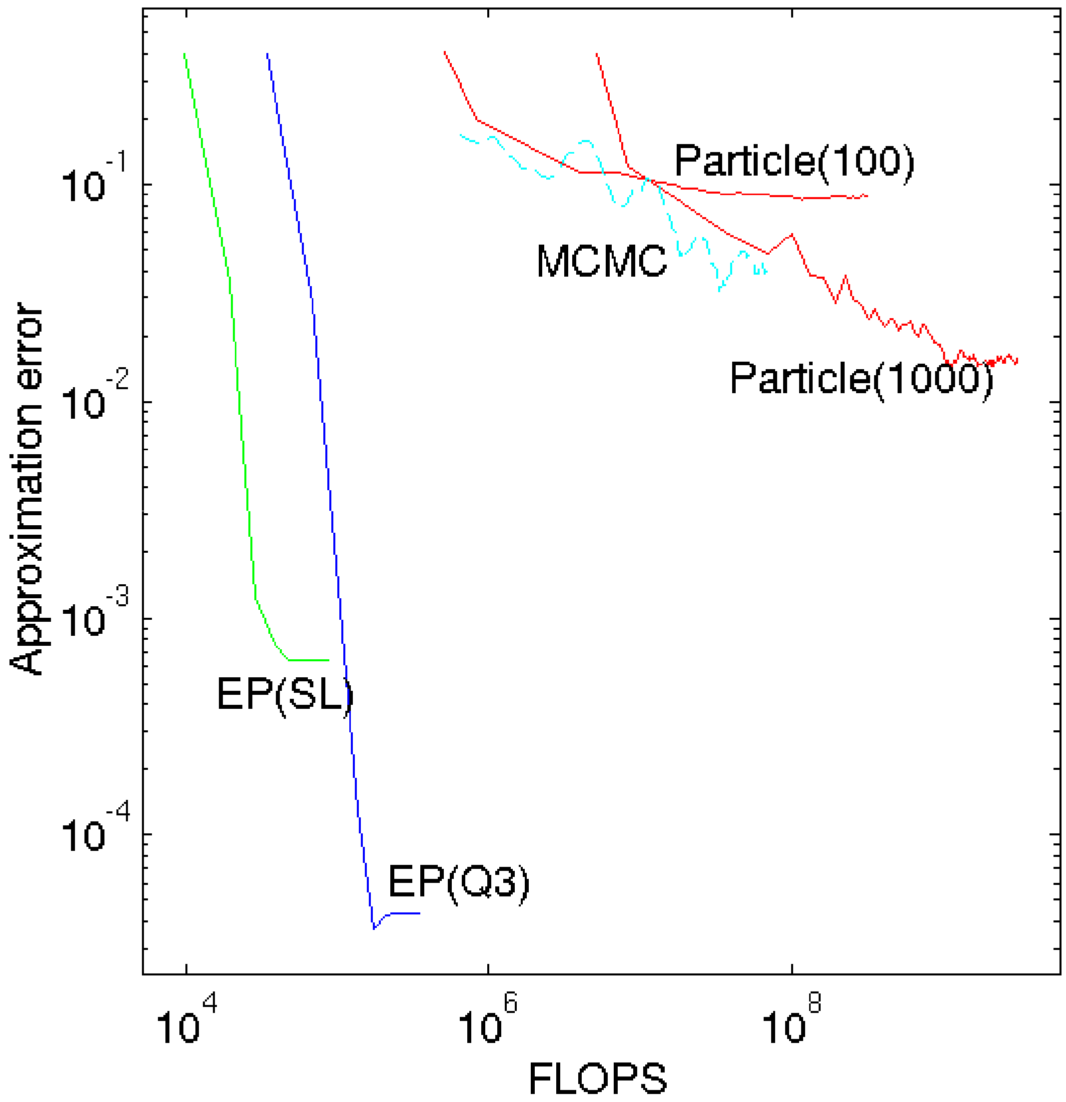
$$N(x_1; m_1, v_1) = \frac{\mathrm{proj}\left[Po(y_1; e^{x_1})\, q_{\triangleleft}(x_1)\right]}{q_{\triangleleft}(x_1)}$$


EP iter 1
EP iter 2
EP iter 10
0.5
0
-0.5
-1
-1.5
State mean
0
20
40
60
80
100
Time index

Posterior for the last state




EP
Exact
Particle(100)
MCMC
State posterior mean
0.5
0
-0.5
-1
0
20
40
60
80
100
Time index
State posterior variance
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0
20
40
60
80
100
Time index

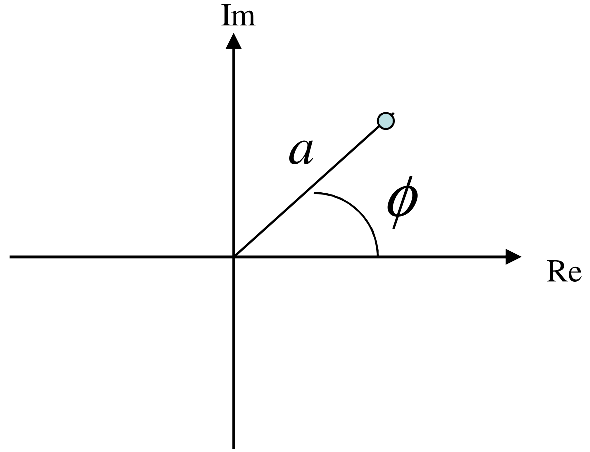


Approximation error
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{4}
10^{6}
10^{8}
FLOPS
Particle(100)
MCMC
Particle(1000)
EP(SL)
EP(Q3)

EP for signal detection

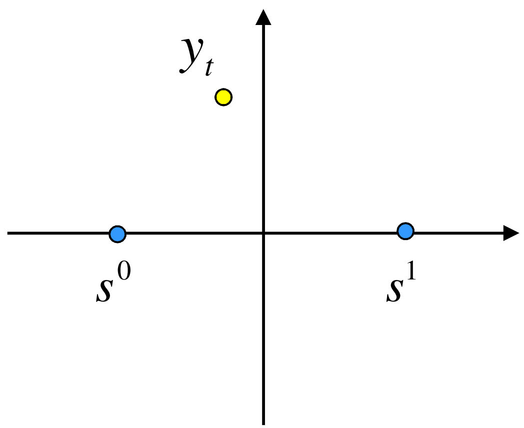
(Qi and Minka, 2003)

- Wireless communication problem
- Transmitted signal = $a\sin(\omega t+\phi)$
- (a,ϕ) vary to encode each symbol
- In complex numbers: $ae^{i\phi}$



Binary symbols, Gaussian noise

- Symbols are $s^1 = 1$ and $s^0 = -1$ (in complex plane)
- Received signal $y_t = a\sin(\omega t + \phi) + \text{noise}$
- Optimal detection is easy in this case

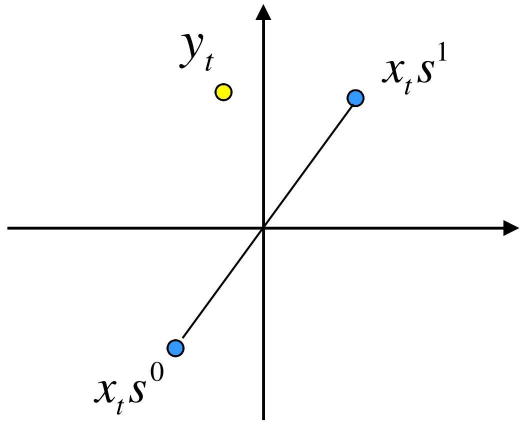


Fading channel

- Channel systematically changes amplitude and phase:

$$y_t = x_t s_t + \text{noise}$$

- s_t = transmitted symbol
- x_t = channel multiplier (complex number)
- x_t changes over time

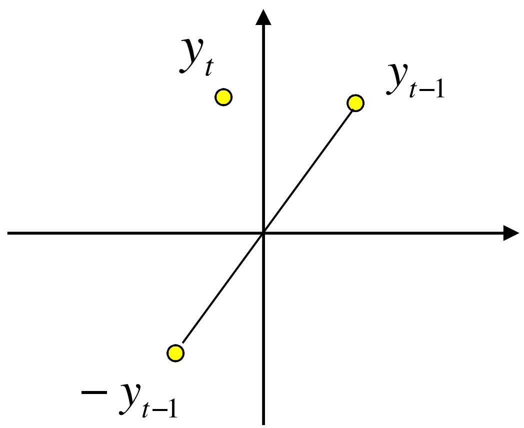


Differential detection

- Use last measurement to estimate state:

$$x_t \approx y_{t-1} / s_{t-1}$$

- State estimate is noisy – can we do better?



Factor graph

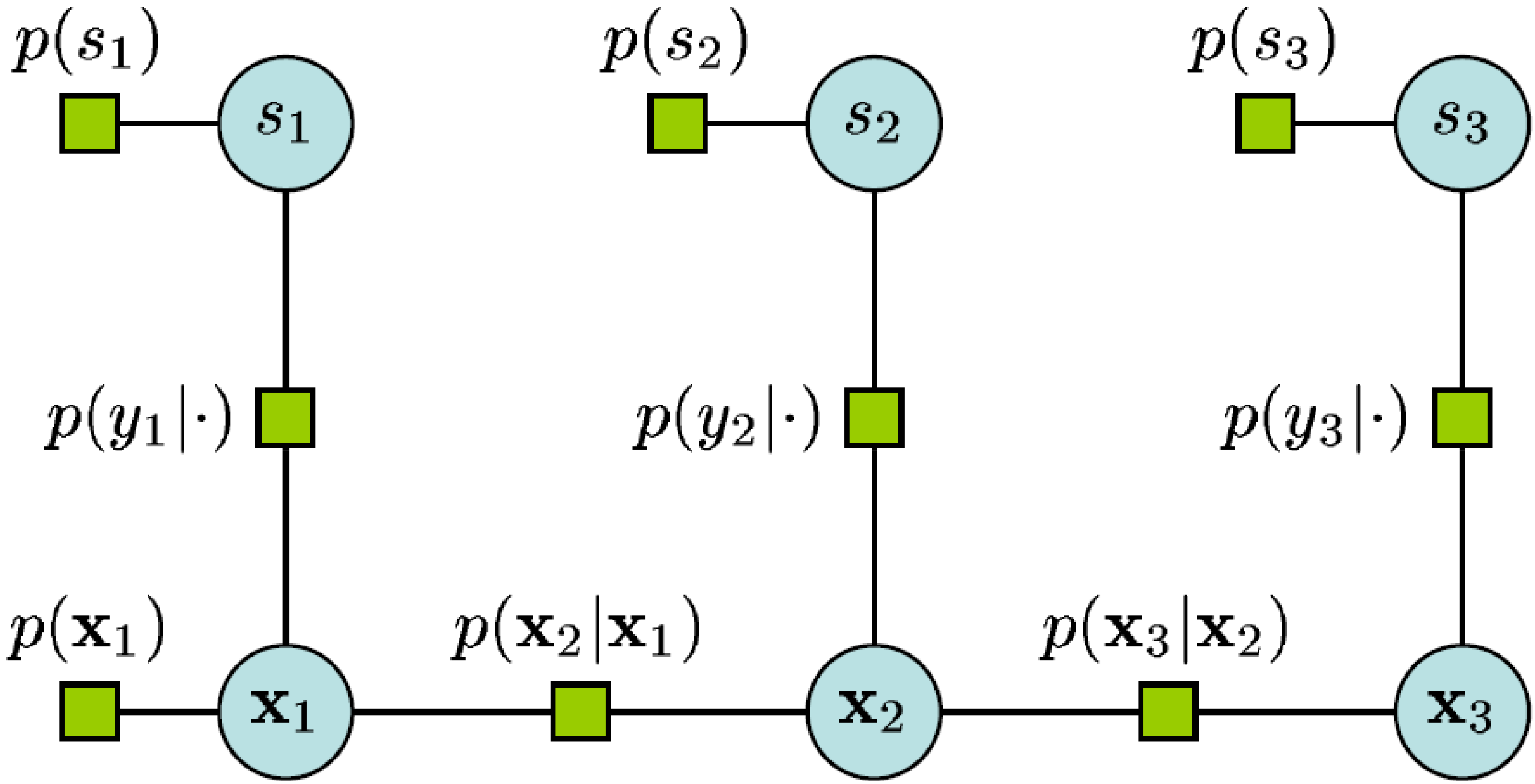
s_1 s_2 s_3 s_4

y_1 y_2 y_3 y_4

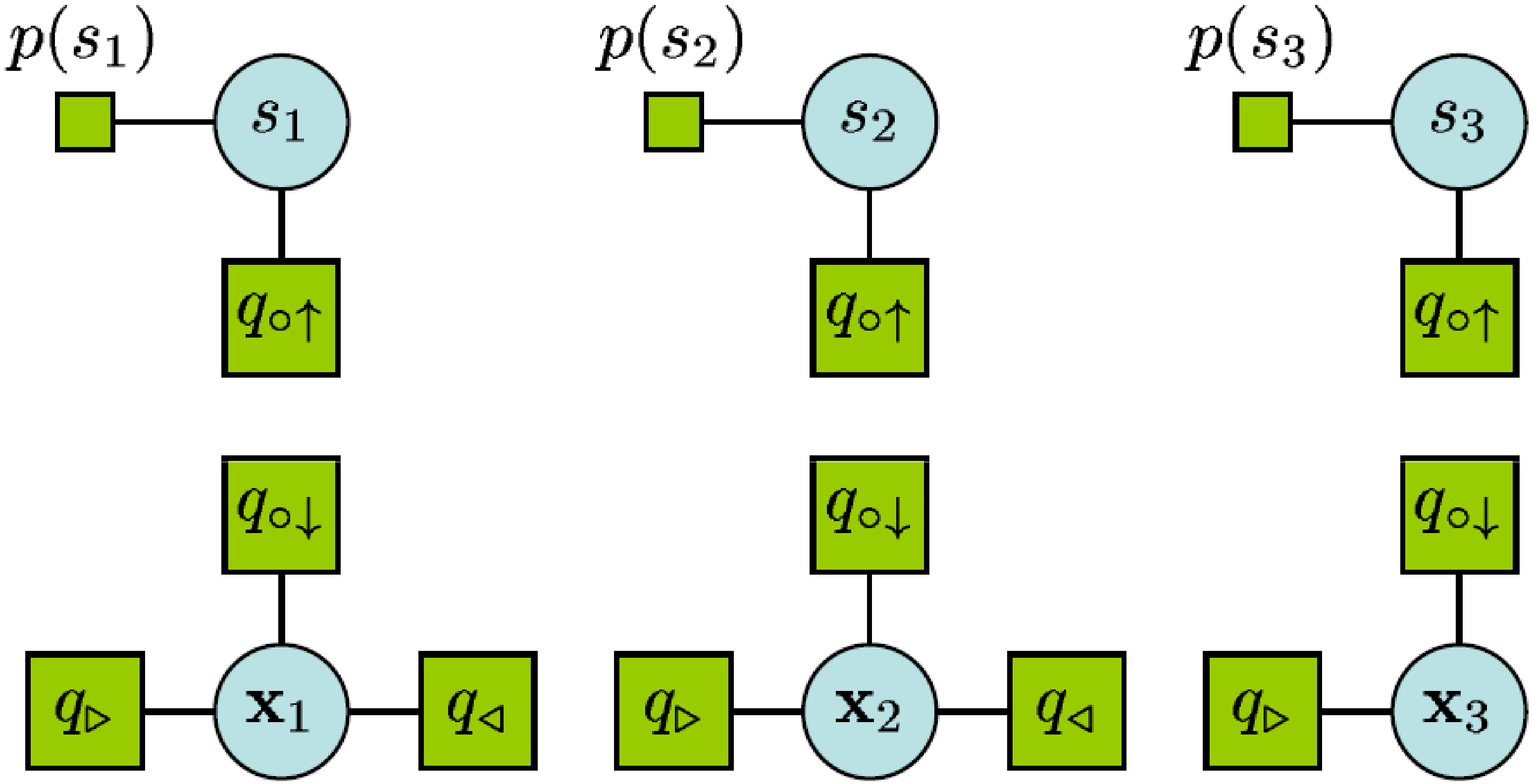
x_1 x_2 x_3 x_4

Symbols can also be correlated (e.g. error-correcting code)

Channel dynamics are learned from training data (all 1's)

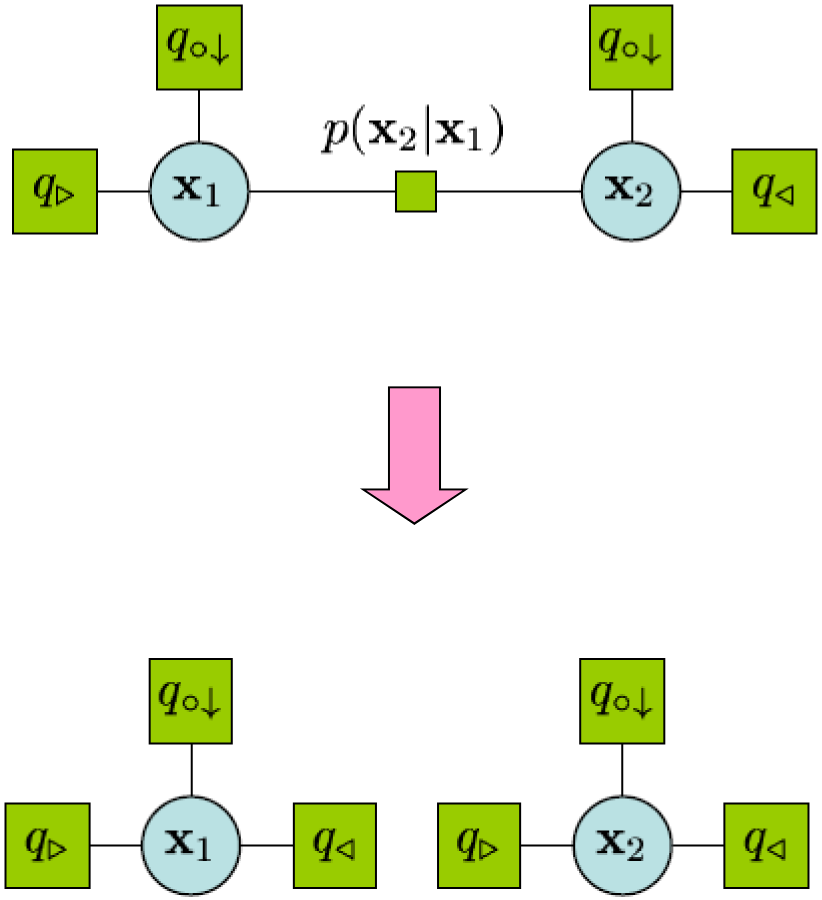


(a) Exact posterior $p(s_1, s_2, s_3, \mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)$

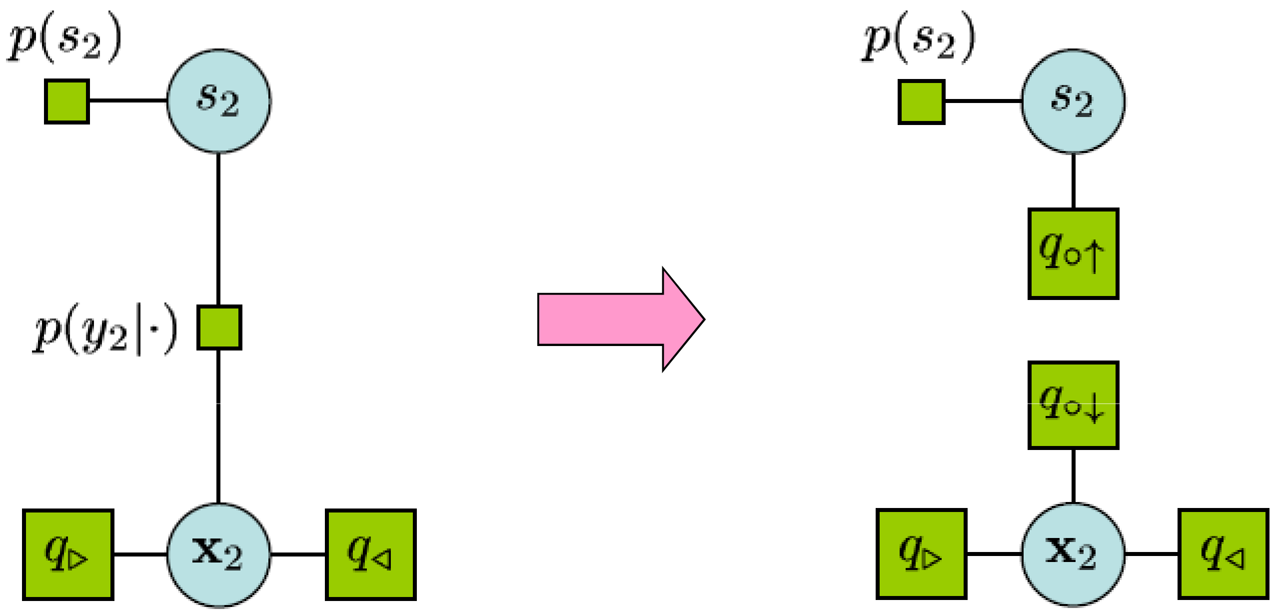


(b) Approximate posterior $\prod_i q(s_i)q(\mathbf{x}_i)$

Splitting a transition factor



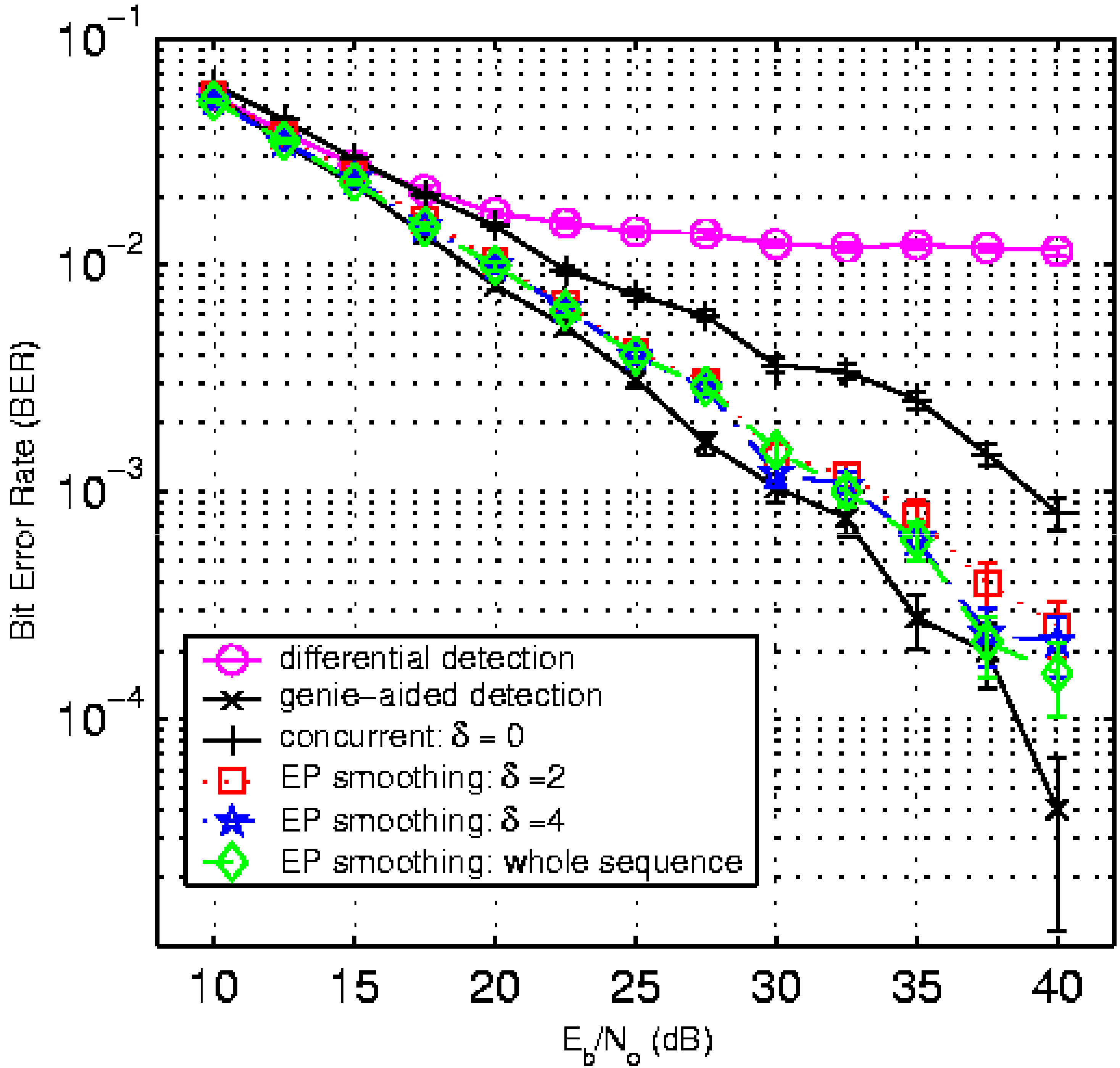
Splitting a measurement factor



On-line implementation

- Iterate over the last δ measurements
- Previous measurements act as prior

- Results comparable to particle filtering, but much faster

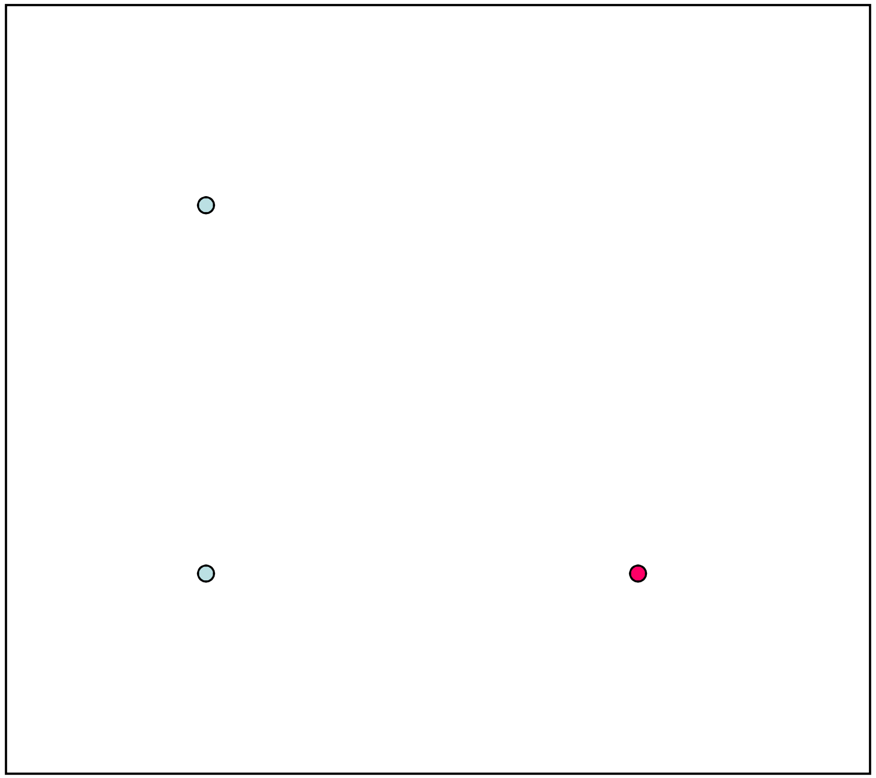


10^{-1}
10^{-2}
10^{-3}
10^{-4}
Bit Error Rate (BER)
10
15
20
25
30
35
40
E_b/N_o (dB)
differential detection
genie–aided detection
concurrent: δ = 0
EP smoothing: δ =2
EP smoothing: δ =4
EP smoothing: whole sequence

Classification problems

Spam filtering by linear separation

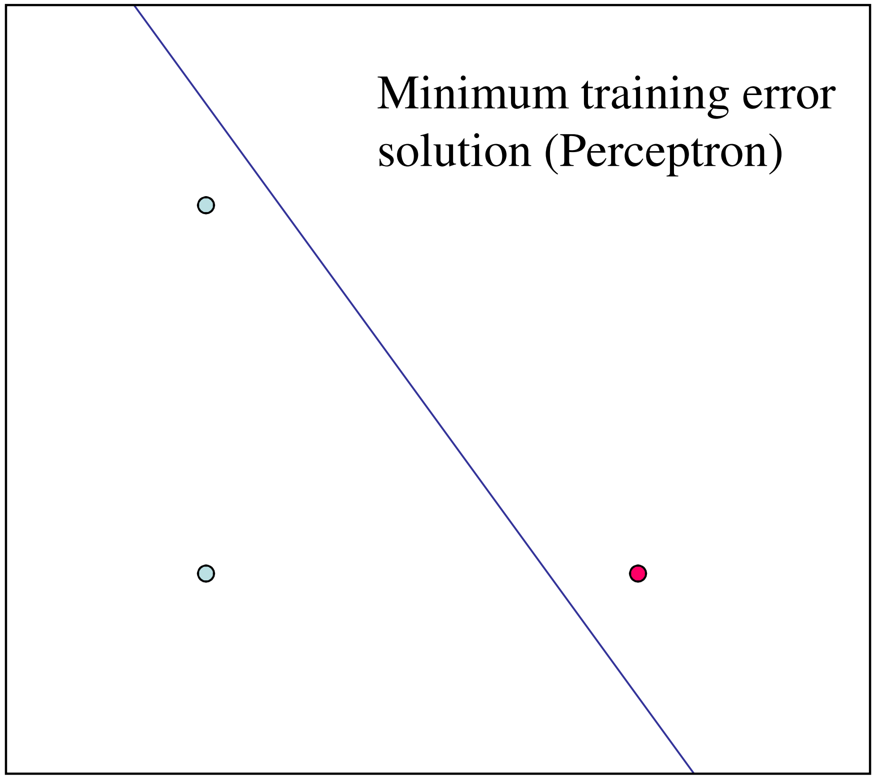
Not spam



Spam

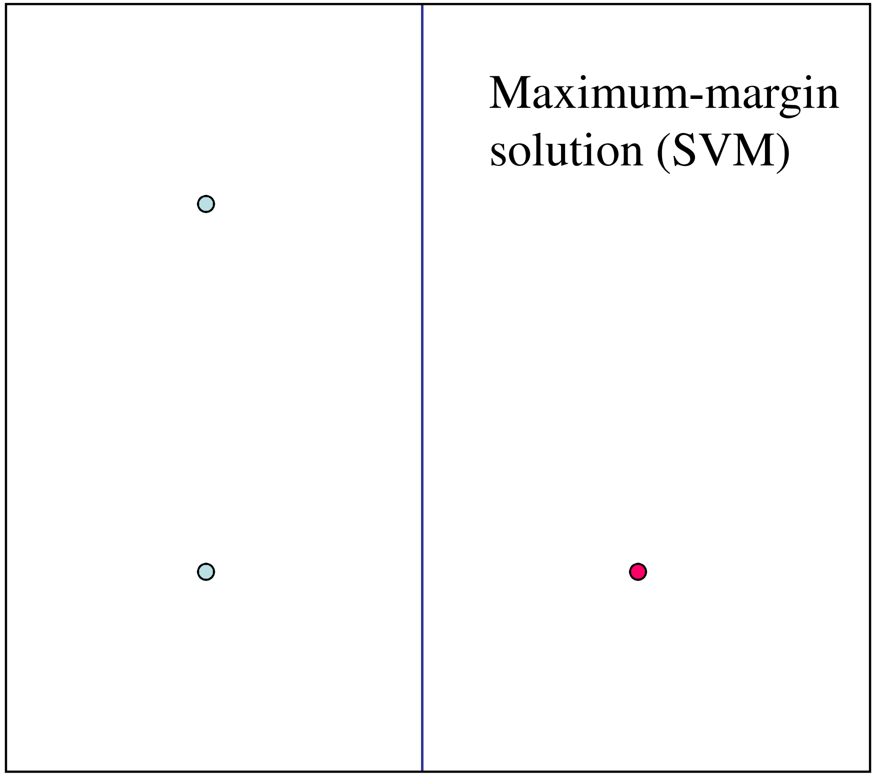
Choose a boundary that will generalize to new data

Linear separation



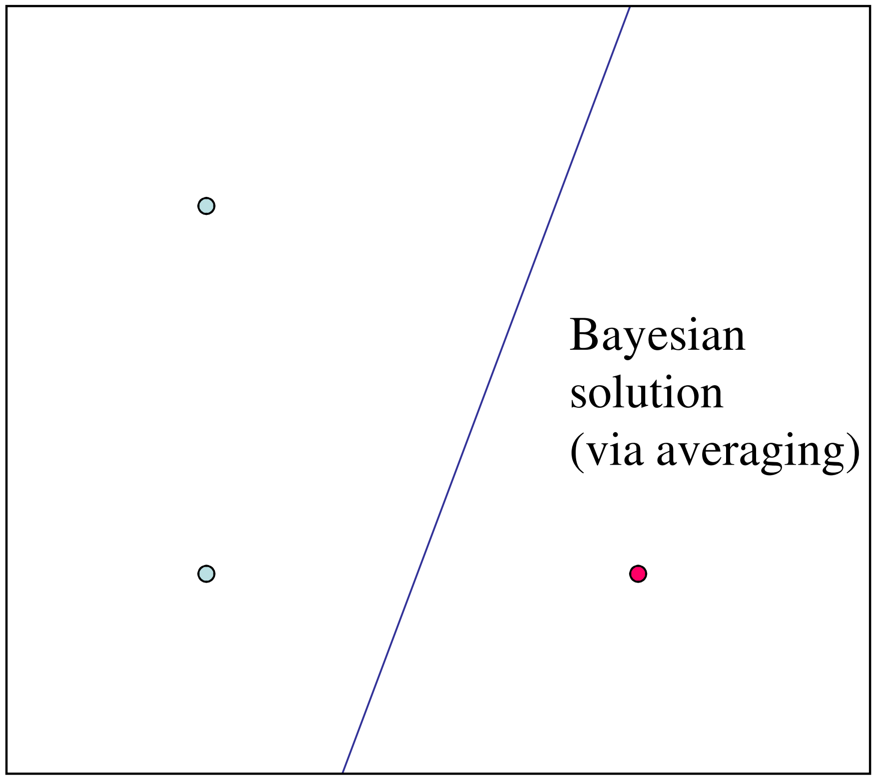
Too arbitrary – won’t generalize well

Linear separation



Ignores information in the vertical direction

Linear separation

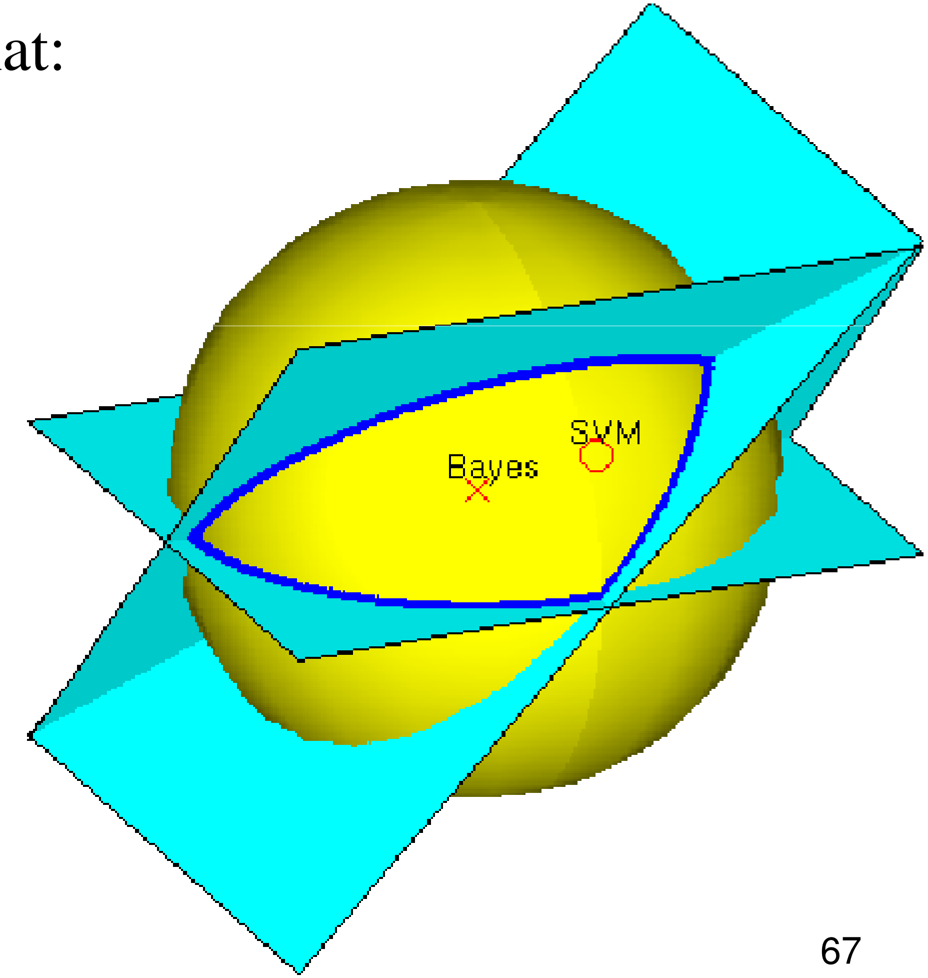


Has a margin, and uses information in all dimensions

Geometry of linear separation

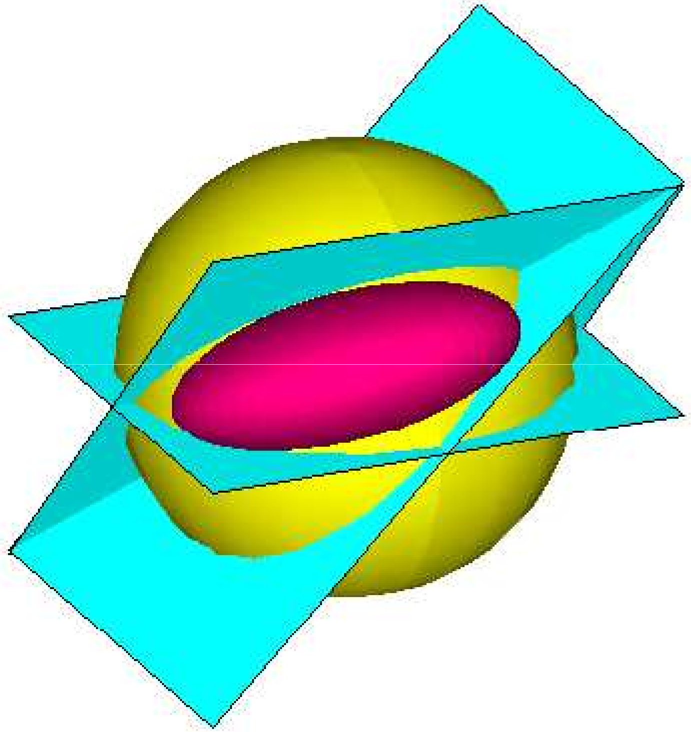
Separator is any vector w such that:

$$\mathbf{w}^T \mathbf{x}_i > 0 \quad \text{(class 1)}$$
$$\mathbf{w}^T \mathbf{x}_i < 0 \quad \text{(class 2)}$$
$$\|\mathbf{w}\| = 1 \quad \text{(sphere)}$$



This set has an unusual shape
SVM: Optimize over it
Bayes: Average over it

Performance on linear separation



EP Gaussian approximation to posterior

Factor graph

$$p(y_i = \pm 1 \mid \mathbf{x}_i, \mathbf{w}) = I(y_i \mathbf{x}_i^\top \mathbf{w} > 0)$$

$$p(\mathbf{w}) = N(\mathbf{w}; \mathbf{0}, \mathbf{I})$$

Computing moments

$$p(y_i = \pm 1 \mid \mathbf{x}_i, \mathbf{w}) = I(y_i \mathbf{x}_i^\top \mathbf{w} > 0)$$

$$q^{\setminus i}(\mathbf{w}) = N(\mathbf{w}; \mathbf{m}^{\setminus i}, \mathbf{V}^{\setminus i})$$

Computing moments

Time vs. accuracy

A typical run on the 3-point problem

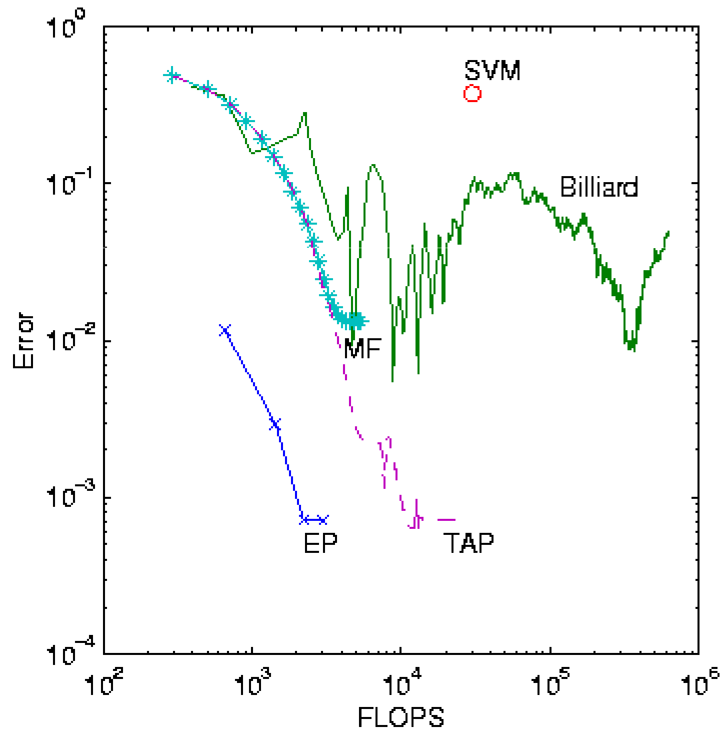
Error = distance to true mean of w

Billiard = Monte Carlo sampling
(Herbrich et al, 2001)

Opper&Winther's algorithms:

MF = mean-field theory

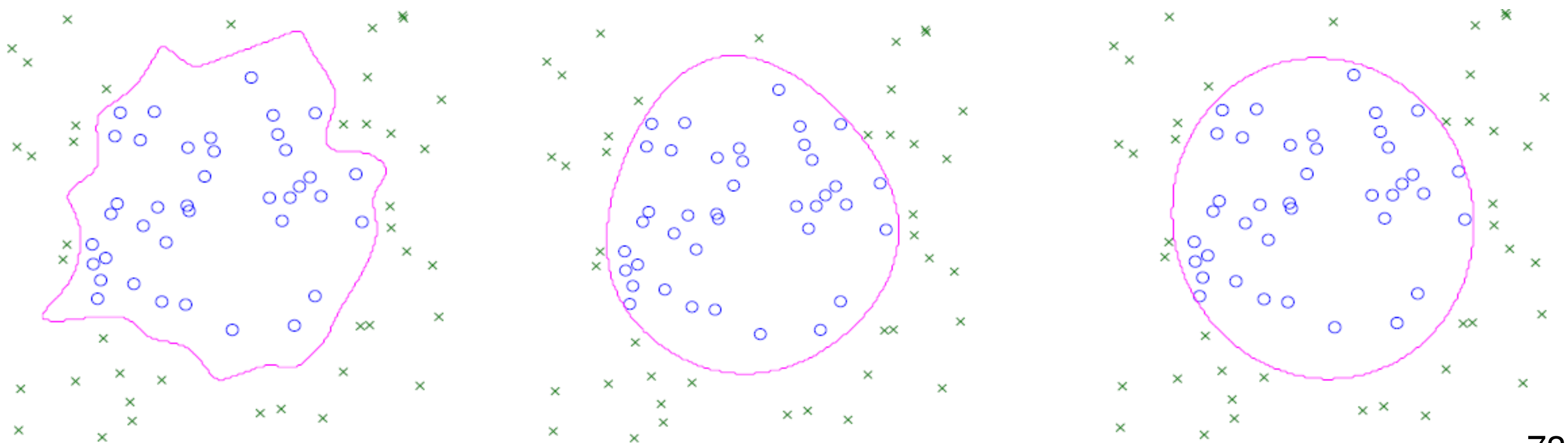
TAP = cavity method (equiv to Gaussian EP for this problem)



Gaussian kernels

- Map data into high-dimensional space so that

$$\phi(\mathbf{x}_i)^{\mathrm{T}}\phi(\mathbf{x}_j) = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2}\right)$$



Bayesian model comparison

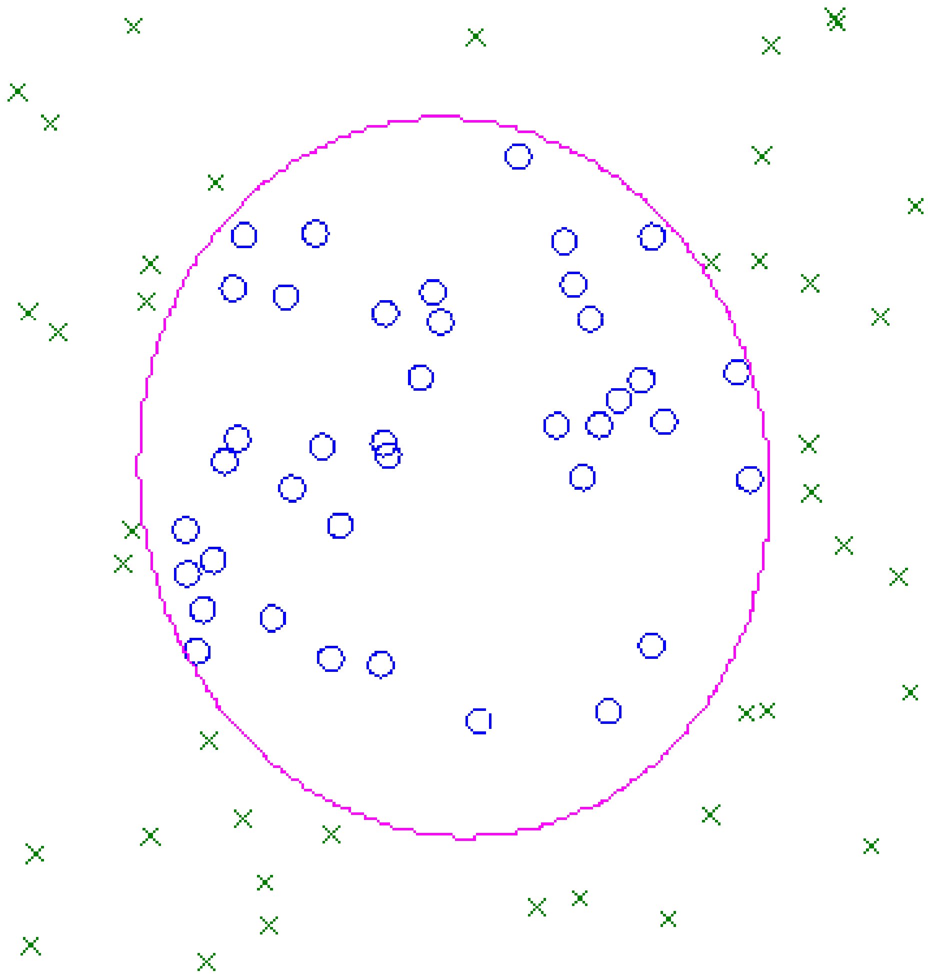
- Multiple models M_i with prior probabilities $p(M_i)$
- Posterior probabilities:

$$p(M_i|D) \propto p(D|M_i)p(M_i)$$

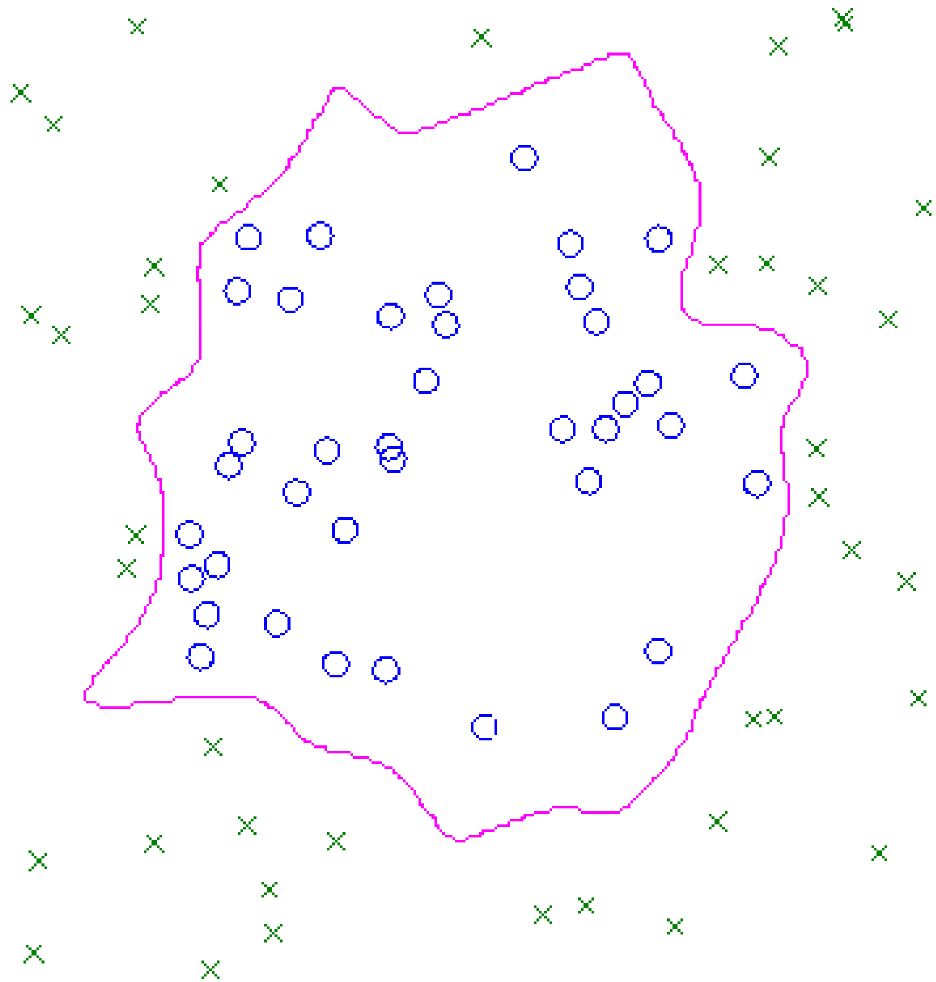
- For equal priors, models are compared using model evidence:

$$p(D|M_i) = \int_\theta p(D,\theta|M_i)d\theta$$

Highest-probability kernel



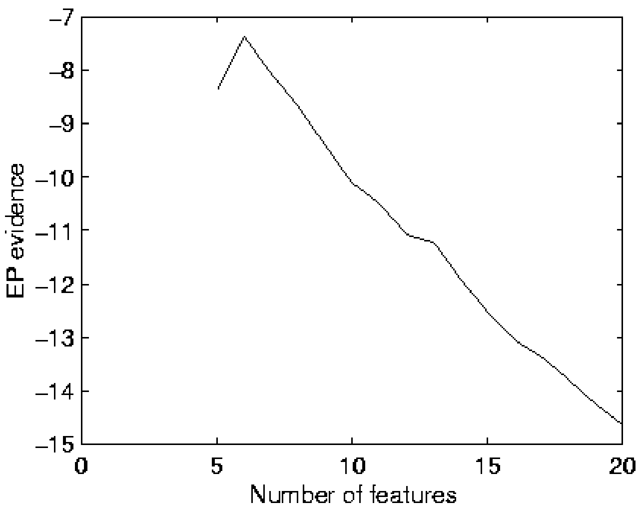
Margin-maximizing kernel



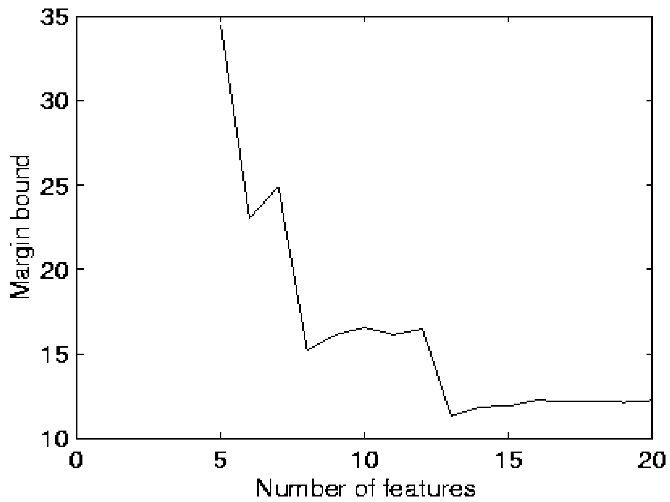
Bayesian feature selection

Synthetic data where 6 features are relevant (out of 20)

Bayes picks 6



Margin picks 13



EP versus Monte Carlo

- Monte Carlo is general but expensive
  - A sledgehammer
- EP exploits underlying simplicity of the problem (if it exists)
- Monte Carlo is still needed for complex problems (e.g. large isolated peaks)
- Trick is to know what problem you have

Software for EP

- Bayes Point Machine toolbox
  http://research.microsoft.com/~minka/papers/ep/bpm/

- Sparse Online Gaussian Process toolbox
  http://www.kyb.tuebingen.mpg.de/bs/people/csatol/ogp/index.html

- Infer.NET
  http://research.microsoft.com/infernet

Further reading

- EP bibliography
  http://research.microsoft.com/~minka/papers/ep/roadmap.html

- EP quick reference
  http://research.microsoft.com/~minka/papers/ep/minka-ep-quickref.pdf

Tomorrow

- Variational Message Passing
- Divergence measures
- Comparisons to EP