Computing Cramér-Rao bounds in graphical models

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Motivation

- Cramér-Rao bounds (CRBs) are lower bounds on MSE of estimators.
- In the case of (deterministic) parameter estimation, the CRBs bound the MSE (mean squared error) of unbiased estimators.
- In the case of random variables, the CRBs bound the MSE of both unbiased and biased estimators.
- CRBs have been computed for estimators of fixed parameters in various contexts, e.g., communications and image processing.
- CRBs have been computed for filtering the state in state space models with freely evolving states [Tichavský et al., 1998], e.g., tracking of slowly varying parameters.
- Extension to
  - cycle-free graphical models, e.g., filtering/smoothing of input/state in general state space models
  - Particular cyclic graphical models, i.e., joint decoding and channel estimation
- In this talk, all proofs are omitted.

Overview

- Introduction to CRBs
- Matrix inversion lemma
- CRBs for estimation in cycle-free graphical models
- State space model
- CRBs for filtering
- CRBs for smoothing
- Examples
- Conclusion

Introduction to CRBs

- Let $p(x, y)$ be the joint probability function of X and Y, where $X^T \triangleq (X_1, X_2, \ldots, X_N)$ and $X_i \in \mathbb{R}^l$;
  thus $X^T = (X_{11}, X_{12}, \ldots, X_{1\ell}, X_{21}, \ldots, X_{2\ell}, \ldots, X_{N\ell})$.
- $\hat{X}(Y)$ is the estimate of X based on the observations Y.
- Error matrix $\mathbf{E} \triangleq \mathrm{E}_{XY}[(\hat{X}(Y) - X)(\hat{X}(Y) - X)^T]$.
- Posterior information matrix $\mathbf{J}(X)$ defined as

$$\mathbf{J}_{ij}(X) \triangleq \mathrm{E}_{XY}\left[\nabla_{x_i} \log p(x, y) \nabla_{x_j}^T \log p(x, y)\right],$$

  under the assumption that $\mathrm{E}_{XY}\left[\nabla_{x_i} \log p(x, y) \nabla_{x_j}^T \log p(x, y)\right]$ exists, $\forall x$ and y.

Introduction to CRBs (2)

Theorem (Fisher, '22; Dugué, '37; Rao, '45; Cramér, '46)

Let $p(x, y)$ be the joint probability function of X and Y and $\mathbf{E}$ the error matrix. If

1. $\nabla_{x_j} p(x, y)$ and $\nabla_{x_i} \nabla_{x_j} p(x, y) = 0$ exist $\forall x$ and y,
2. the posterior information matrix $\mathbf{J}(X)$ exists and is non-singular,
3. $\int_x \nabla_{x_j} [B(x)p(x)] = 0$, where $B(x) = \int_y [\hat{x}(y) - x] p(y|x) dy$,

then $\mathbf{E} \succeq \mathbf{J}(X)^{-1}$.

In words
$\mathbf{D} \triangleq \mathbf{E} - \mathbf{J}(X)^{-1}$ is positive semi-definite, i.e., $v^T \mathbf{D} v \geq 0, \forall v \in \mathbb{R}^{lN}$.

Notice that the estimators are not necessarily unbiased!
The assumption (3) is weaker.

Introduction to CRBs (5)

Posterior information matrix $\mathbf{J}(X)$ can be computed in several ways

$$
\begin{aligned}
\mathbf{J}_{ij}(X) &\stackrel{\triangle}{=} \mathrm{E}_{XY}\left[\nabla_{x_i}\log p(x,y)\nabla^T_{x_j}\log p(x,y)\right] \\
&\stackrel{\text{(L1)}}{=} -\mathrm{E}_{XY}\left[\nabla_{x_i}\nabla^T_{x_j}\log p(x,y)\right] \\
&= -\mathrm{E}_{XY}\left[\nabla_{x_i}\nabla^T_{x_j}\log p(y|x)\right] - \mathrm{E}_{X}\left[\nabla_{x_i}\nabla^T_{x_j}\log p(x)\right] \\
&\stackrel{\text{(L2 \& L3)}}{=} \mathrm{E}_{XY}\left[\nabla_{x_i}\log p(y|x)\nabla^T_{x_j}\log p(y|x)\right] + \mathrm{E}_{X}\left[\nabla_{x_i}\log p(x)\nabla^T_{x_j}\log p(x)\right]
\end{aligned}
$$

Introduction to CRBs (4)

Corollaries

Since $\mathbf{D} \triangleq \mathbf{E} - \mathbf{J}^{-1}$ is positive semi-definite, i.e., $x^T \mathbf{D} x \geq 0, \forall \boldsymbol{x} \in \mathbb{R}^{lN}$, it follows

- $\mathbf{E}_{ii} = \mathrm{E}_{p(x_i,y)}[(\hat{X}_i(Y) - X_i)(\hat{X}_i(Y) - X_i)^T] \succeq [\mathbf{J}(X)^{-1}]_{ii}$

  Proof: Set $x = [0, \ldots, 0, x_i, 0]^T$.

- $E_{ij,ij} = \mathrm{E}_{p(x_{ij},y)}[(\hat{X}_{ij}(Y) - X_{ij})^2] \geq [\mathbf{J}(X)^{-1}]_{ij,ij}$.

  Proof: Set $x = [0, \ldots, 0, x_{ij}, 0]^T$.

- $\mathrm{Tr}[\mathbf{E} - \mathbf{J}^{-1}] \geq 0$, hence $\mathrm{Tr}[\mathbf{E}] \triangleq \sum_{i,j} \mathrm{E}[(\hat{X}_{ij} - X_{ij})^2] \geq \mathrm{Tr}[\mathbf{J}(X)^{-1}]$.

- $\sum_i \mathrm{E}[(\hat{X}_{ij} - X_{ij})^2] \geq \sum_i [\mathbf{J}(X)^{-1}]_{ij}$.

Observation

We need to invert $\mathbf{J}(X)$! However, we only need the diagonal elements of $\mathbf{J}(X)^{-1}$.

If $\mathbf{J}(X)$ is sparse, the inversion can be done efficiently by matrix inversion lemma.

This is can be viewed as message passing.

Matrix inversion lemma

Let $\mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix}$, where $\mathbf{A}_{11}$ and $\mathbf{A}_{22}$ are nonsingular, such that $(\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{21})$ and $(\mathbf{A}_{11} - \mathbf{A}_{22}\mathbf{A}_{11}^{-1}\mathbf{A}_{12})$ are also nonsingular.

Then $\mathbf{A}$ is also nonsingular with

$$\begin{aligned}
[\mathbf{A}^{-1}]_{11} &= \mathbf{A}_{11}^{-1} + \mathbf{A}_{11}^{-1}\mathbf{A}_{12}(\mathbf{A}_{22} - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12})^{-1}\mathbf{A}_{21}\mathbf{A}_{11}^{-1} \\
&= (\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{21})^{-1}
\end{aligned}$$

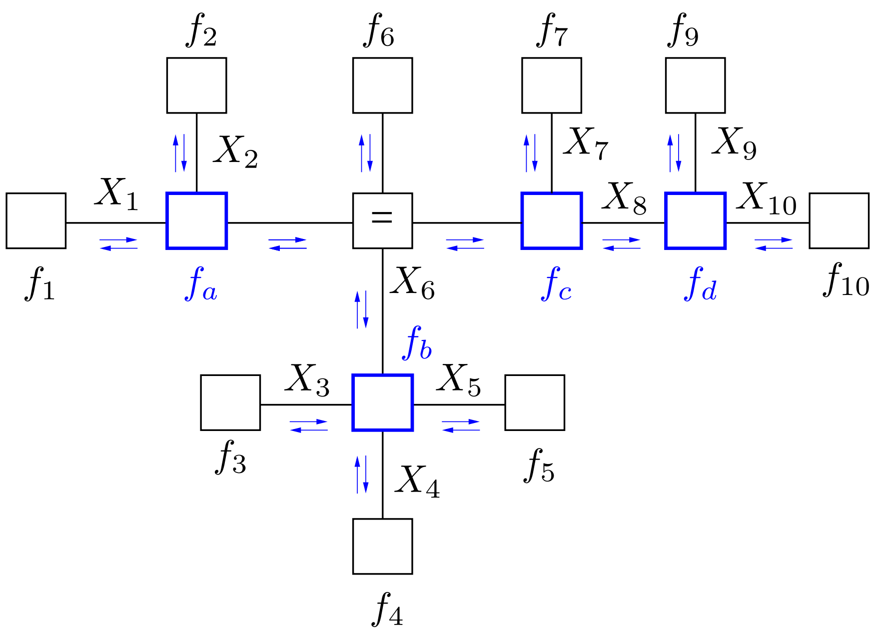
$$\begin{aligned}
[\mathbf{A}^{-1}]_{12} &= -\mathbf{A}_{11}^{-1}\mathbf{A}_{12}(\mathbf{A}_{22} - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12})^{-1} \\
&= -(\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{21})^{-1}\mathbf{A}_{12}\mathbf{A}_{22}^{-1}
\end{aligned}$$

$$\begin{aligned}
[\mathbf{A}^{-1}]_{21} &= -(\mathbf{A}_{22} - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12})^{-1}\mathbf{A}_{21}\mathbf{A}_{11}^{-1} \\
&= -\mathbf{A}_{22}^{-1}\mathbf{A}_{21}(\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{21})^{-1}
\end{aligned}$$

$$\begin{aligned}
[\mathbf{A}^{-1}]_{22} &= \mathbf{A}_{22}^{-1} + \mathbf{A}_{22}^{-1}\mathbf{A}_{21}(\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{21})^{-1}\mathbf{A}_{12}\mathbf{A}_{22}^{-1} \\
&= (\mathbf{A}_{22} - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12})^{-1}.
\end{aligned}$$

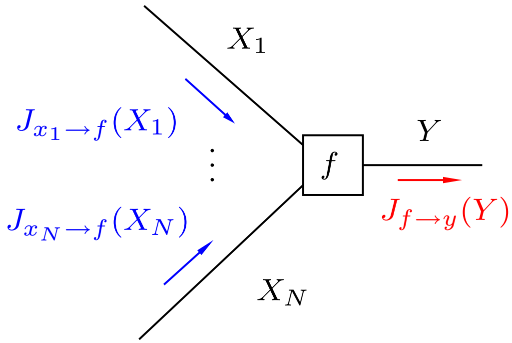
CRB for estimation in graphical models

- The posterior CRBs of variables in cycle-free graphical models can be computed efficiently by message passing.
- The messages are matrices (or sometimes scalars).
- The messages are updated at each node according to a specific update rule.
- The posterior CRBs are computed by combining those messages, similarly as the computation of marginals.



CRB for estimation in graphical models (2)

Update rule



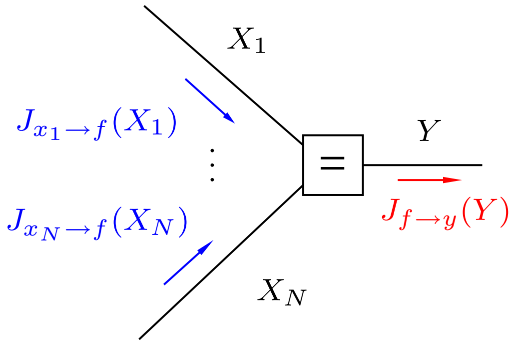
$$J^{-1}_{f \to y}(Y) = \left(\begin{bmatrix} J_{x_1 \to f}(X_1) + \mathrm{E}[-\Delta_{x_1}^{x_1} \log f] & \dots & \mathrm{E}[-\Delta_{x_1}^{x_N} \log f] & \mathrm{E}[-\Delta_{x_1}^{y} \log f] \\ \vdots & \dots & \dots & \vdots \\ \mathrm{E}[-\Delta_{x_N}^{x_1} \log f] & \dots & J_{x_N \to f}(X_N) + \mathrm{E}[-\Delta_{x_N}^{x_N} \log f] & \mathrm{E}[-\Delta_{x_N}^{y} \log f] \\ \mathrm{E}[-\Delta_{y}^{x_1} \log f] & \dots & \mathrm{E}[-\Delta_{y}^{x_N} \log f] & \mathrm{E}[-\Delta_{y}^{y} \log f] \end{bmatrix}^{-1} \right)_{N+1, N+1}$$

Remark:

- The expectations $\mathrm{E}[\Delta_{x_i}^{x_j} \log f]$ are supposed to be computable.
- One can exchange rows and corresponding columns in the above matrix, it leads to the same $J_{f \to y}(Y)$.

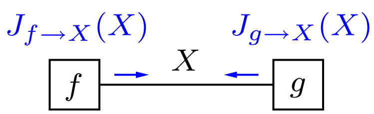
CRB for estimation in graphical models (3)

Update rule



$$J_{f \to y}(Y) = \sum_{i=1}^{N} J_{x_i \to f}(X_i)$$

Posterior CRB



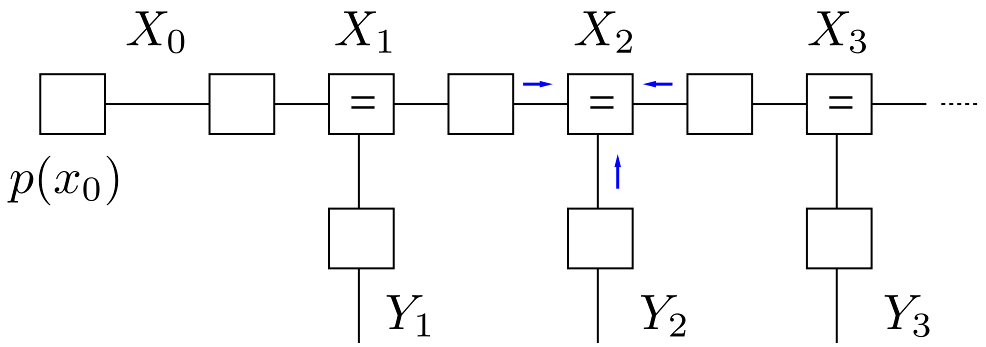
$$J(X) = J_{f \to X}(X) + J_{g \to X}(X)$$

State space model (I)

- Assume $p(x, y)$ factorizes as

$$p(x, y) = p(x_0) \prod_{k=1}^{N} p(x_k | x_{k-1}) p(y_k | x_k).$$

- Freely evolving state X.
- The marginals $p(x_k)$ can be computed by message passing.
- The CRBs can be computed similarly, i.e., by forward and backward sweep!



CRB for filtering

Theorem [Tichavský et al., 1998] ("forward sweep")

$$\mathbf{J}(X_{k+1}) = \mathbf{J}^U(X_{k+1}) + \mathbf{D}_k^{22} - \mathbf{D}_k^{21}(\mathbf{J}(X_k) + \mathbf{D}_k^{11})^{-1}\mathbf{D}_k^{12},$$

where

$$\begin{aligned}
\mathbf{D}_k^{11} &= \mathrm{E}[-\Delta_{x_k}^{x_k} \log p(x_{k+1}|x_k)] \\
\mathbf{D}_k^{12} &= [D_k^{21}]^T = \mathrm{E}[-\Delta_{x_k}^{x_{k+1}} \log p(x_{k+1}|x_k)] \\
\mathbf{D}_k^{22} &= \mathrm{E}[-\Delta_{x_{k+1}}^{x_{k+1}} \log p(x_{k+1}|x_k)] \\
\mathbf{J}^U(X_{k+1}) &= \mathrm{E}[-\Delta_{x_{k+1}}^{x_{k+1}} \log p(y_{k+1}|x_{k+1})] \\
\Delta_x^y &= \nabla_x \nabla_y^T \\
J(X_k) &\triangleq \left[\mathbf{J}(X_1^k)^{-1}\right]_{kk} \\
X_s^t &= (X_s, X_{s+1}, \ldots, X_t) \qquad (t > s;\, t, s \in \mathbb{N}).
\end{aligned}$$

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CRB for smoothing

Forward Sweep:

$$\mathbf{J}^F(X_{k+1}) = \mathbf{J}^U(X_{k+1}) + \mathbf{D}_k^{22} - \mathbf{D}_k^{21}(\mathbf{J}^F(X_k) + \mathbf{D}_k^{11})^{-1}\mathbf{D}_k^{12} = \mathbf{J}^U(X_{k+1}) + \tilde{\mathbf{J}}^F(X_{k+1}).$$

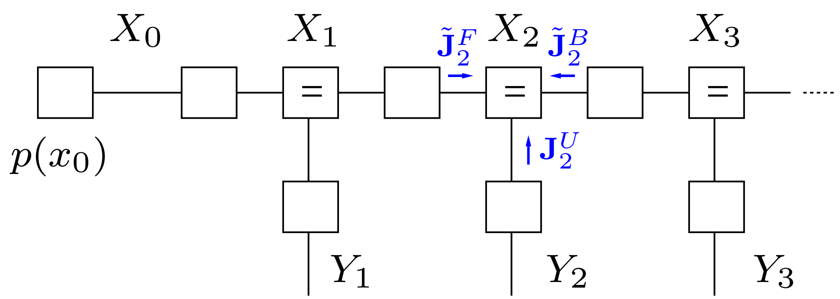
Initialization: $\mathbf{J}^F(X_0) = \mathrm{E}[-\Delta_{x_0}^{x_0} \log p(x_0)]$

Backward Sweep:

$$\mathbf{J}^B(X_{k-1}) = \mathbf{J}^U(X_{k-1}) + \mathbf{D}_{k-1}^{11} - \mathbf{D}_{k-1}^{12}(\mathbf{J}^B(X_k) + \mathbf{D}_{k-1}^{22})^{-1}\mathbf{D}_{k-1}^{21} = \mathbf{J}^U(X_{k-1}) + \tilde{\mathbf{J}}^B(X_{k-1}).$$

Initialization: $\mathbf{J}^B(X_N) = \mathrm{E}[-\Delta_{x_N}^{x_N} \log p(y_N|x_N)] = \mathbf{J}^U(X_N)$

Posterior CRB: $\mathbf{J}^{\text{tot}}(X_k) = \tilde{\mathbf{J}}^F(X_k) + \tilde{\mathbf{J}}^B(X_k) + \mathbf{J}^U(X_k).$

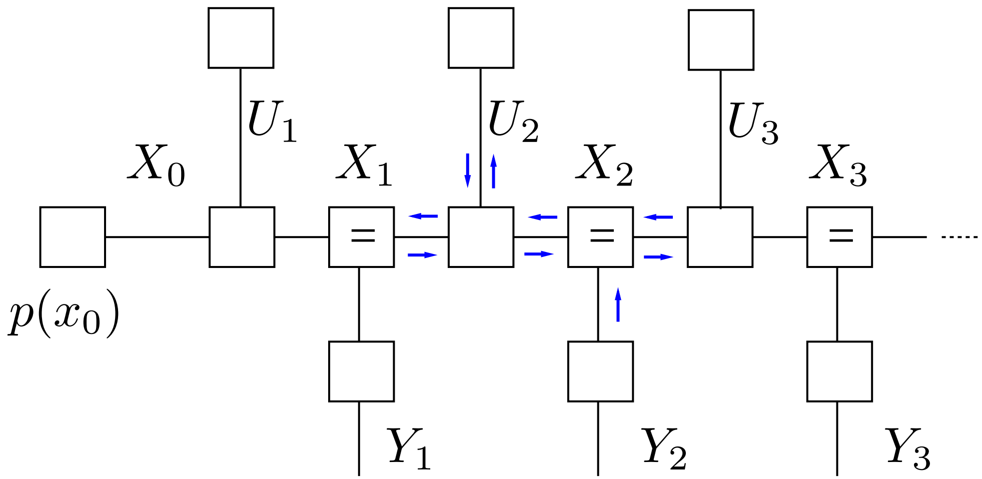


State space model (II)

- Assume $p(x, y, u)$ factorizes as

$$p(x, y, u) = p(x_0) \prod_{k=1}^{N} p(x_k | u_k, x_{k-1}) p(y_k | x_k) p(u_k).$$

- CRB for input U_k and/or state X_k.
- The marginals $p(u_k)$ and $p(x_k)$ can be computed by message passing.
- The CRBs can be computed similarly, i.e., by forward and backward sweep!



CRB for filtering

Theorem ("forward sweep")

$\mathbf{J}(X_{k+1}) = \mathbf{J}^U(X_{k+1}) + \boldsymbol{\zeta}_k^{22} - \boldsymbol{\zeta}_k^{21}(\boldsymbol{\zeta}_k^{11})^{-1}\boldsymbol{\zeta}_k^{12}$, where

$$\begin{aligned}
\boldsymbol{\zeta}_k^{11} &= \mathbf{J}^D(U_{k+1}) + \mathbf{D}_k^{22} - \mathbf{D}_k^{21}(\mathbf{J}(X_k) + \mathbf{D}_k^{11})^{-1}\mathbf{D}_k^{21} \\
\boldsymbol{\zeta}_k^{12} &= \mathbf{D}_k^{23} - \mathbf{D}_k^{21}(\mathbf{J}(X_k) + \mathbf{D}_k^{11})^{-1}\mathbf{D}_k^{31} \\
\boldsymbol{\zeta}_k^{21} &= \mathbf{D}_k^{32} - \mathbf{D}_k^{31}(\mathbf{J}(X_k) + \mathbf{D}_k^{11})^{-1}\mathbf{D}_k^{21} = (\boldsymbol{\zeta}_k^{12})^T \\
\boldsymbol{\zeta}_k^{22} &= \mathbf{D}_k^{33} - \mathbf{D}_k^{31}(\mathbf{J}(X_k) + \mathbf{D}_k^{11})^{-1}\mathbf{D}_k^{31}
\end{aligned}$$

$$\begin{aligned}
\mathbf{D}_k^{11} &= \mathrm{E}[-\Delta_{x_k}^{x_k} \log p(x_{k+1}|u_{k+1}, x_k)] \\
\mathbf{D}_k^{12} &= \mathrm{E}[-\Delta_{x_k}^{u_{k+1}} \log p(x_{k+1}|u_{k+1}, x_k)] = (\mathbf{D}_k^{21})^T \\
\mathbf{D}_k^{13} &= \mathrm{E}[-\Delta_{x_k}^{x_{k+1}} \log p(x_{k+1}|u_{k+1}, x_k)] = (\mathbf{D}_k^{31})^T \\
\mathbf{D}_k^{22} &= \mathrm{E}[-\Delta_{u_{k+1}}^{u_{k+1}} \log p(x_{k+1}|u_{k+1}, x_k)] \\
\mathbf{J}^D(U_{k+1}) &\triangleq \mathrm{E}[-\Delta_{u_{k+1}}^{u_{k+1}} \log p(u_{k+1})] \\
\mathbf{D}_k^{23} &= \mathrm{E}[-\Delta_{u_{k+1}}^{x_{k+1}} \log p(x_{k+1}|u_{k+1}, x_k)] = (\mathbf{D}_k^{32})^T \\
\mathbf{D}_k^{33} &= \mathrm{E}[-\Delta_{x_{k+1}}^{x_{k+1}} \log p(x_{k+1}|u_{k+1}, x_k)] \\
\mathbf{J}^U(X_{k+1}) &\triangleq \mathrm{E}[-\Delta_{x_{k+1}}^{x_{k+1}} \log p(y_{k+1}|x_{k+1})]
\end{aligned}$$

CRB for smoothing

Forward sweep

$$\mathbf{J}^F(X_{k+1}) = \mathbf{J}^U(X_{k+1}) + \boldsymbol{\zeta}_k^{22} - \boldsymbol{\zeta}_k^{21}(\boldsymbol{\zeta}_k^{11})^{-1}\boldsymbol{\zeta}_k^{12} = \mathbf{J}^U(X_{k+1}) + \tilde{\mathbf{J}}^F(X_{k+1})$$

Initialization

$$\mathbf{J}^F(X_0) = \mathrm{E}[-\Delta_{x_0}^{x_0} \log p(x_0)]$$

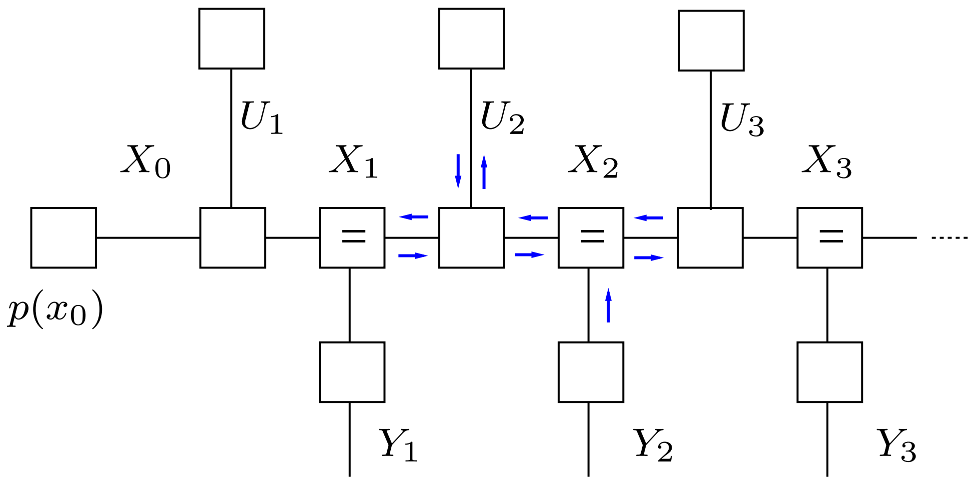
Backward sweep

$$\mathbf{J}^B(X_k) = \mathbf{J}^U(X_k) + \boldsymbol{\rho}_k^{11} - \boldsymbol{\rho}_k^{12}(\boldsymbol{\rho}_k^{22})^{-1}\boldsymbol{\rho}_k^{21} = \mathbf{J}^U(X_k) + \tilde{\mathbf{J}}^B(X_k)$$

Initialization

$$\mathbf{J}(X_N) = \mathbf{J}^U(X_N)$$

Posterior CRB: $\mathbf{J}^{\mathrm{tot}}(X_k) = \tilde{\mathbf{J}}^F(X_k) + \tilde{\mathbf{J}}^B(X_k) + \mathbf{J}^U(X_k).$

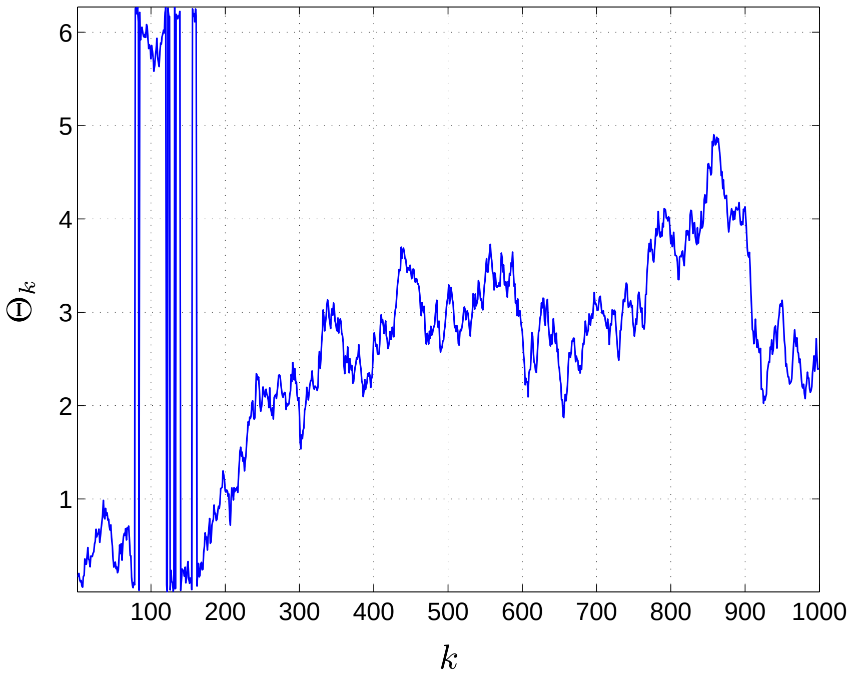


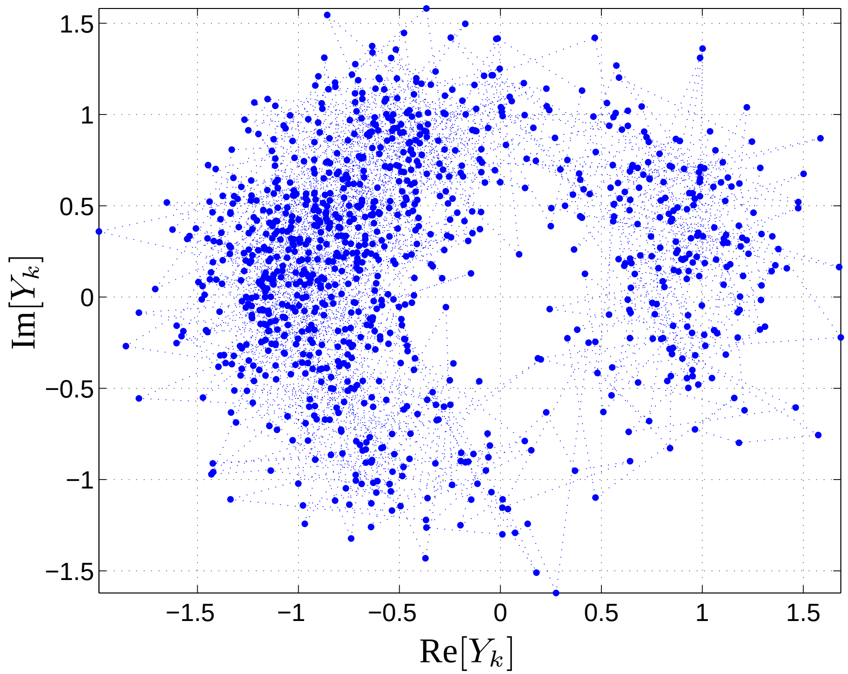
Example 1

Random walk phase model

$$\Theta_{k+1} = (\Theta_k + W_k) \bmod 2\pi$$
$$Y_k = \exp(j\Theta_k) + V_k,$$

where W_k and V_k are i.i.d. (mean free) Gaussian RVs with variance σ_θ^2 and $2\sigma_0^2$ resp.



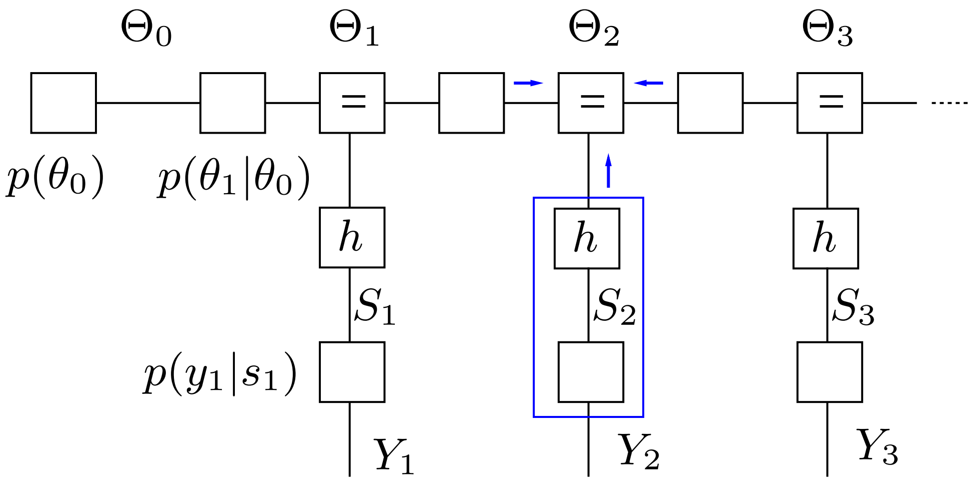


Example 1 (2)

Random walk phase model

$$\Theta_{k+1} = (\Theta_k + W_k) \bmod 2\pi$$
$$Y_k = \exp(j\Theta_k) + V_k,$$

where W_k and V_k are i.i.d. (mean free) Gaussian RVs with variance σ_θ^2 and $2\sigma_0^2$ resp.



$S_i \triangleq \exp(j\Theta_i)$

$h(\theta_k, s_k) \triangleq \delta(s_k - \exp(j\theta_k))$

$p(y_k|s_k) \triangleq (2\pi\sigma_N^2)^{-1} \; \exp(-||y_k - s_k||^2/2\sigma_N^2)$

$p(\theta_k|\theta_{k-1}) \triangleq (2\pi\sigma_W^2)^{-1/2} \; \sum_{n\in\mathbb{Z}} \exp(-((\theta_k - \theta_{k-1}) + n2\pi)^2/2\sigma_W^2).$

Example 1 (3)

Random walk phase model

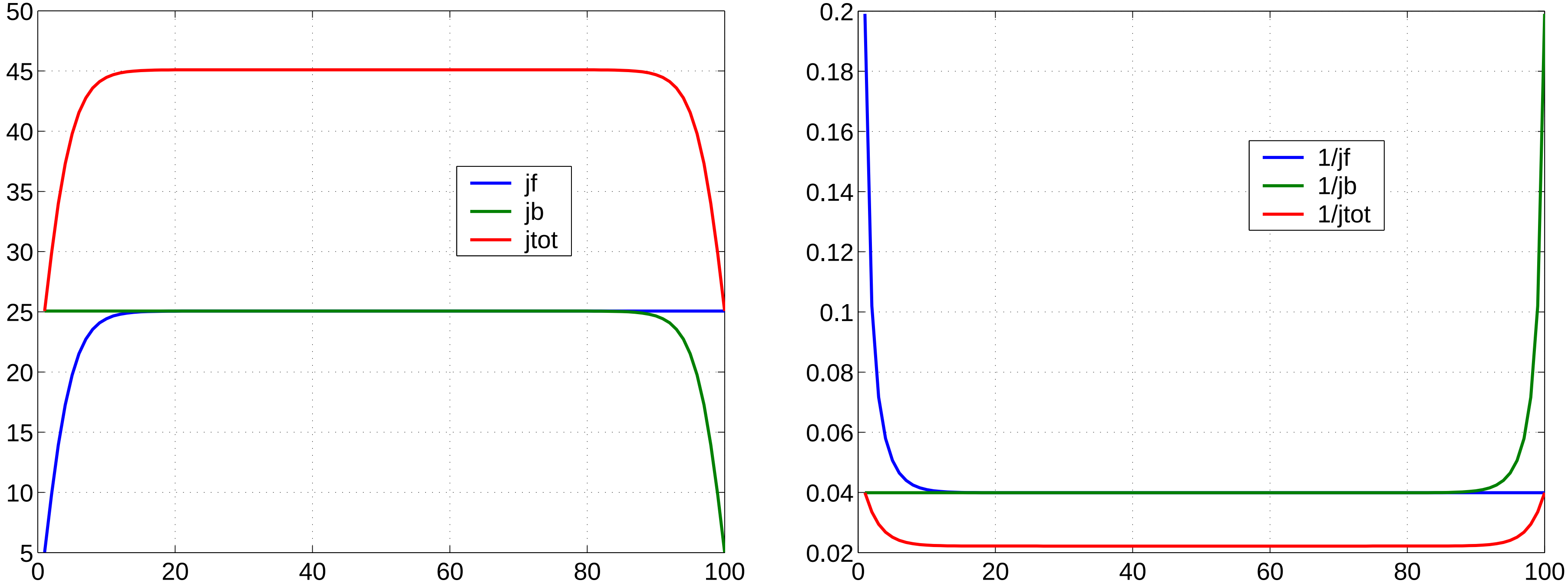
$$\begin{aligned} \Theta_{k+1} &= (\Theta_k + W_k) \bmod 2\pi \\ Y_k &= \exp(j\Theta_k) + V_k, \end{aligned}$$

where W_k and V_k are i.i.d. (mean free) Gaussian RVs with variance σ_θ^2 and $2\sigma_0^2$ resp.

$$\begin{aligned} J^F(\Theta_{k+1}) &= J^U(\Theta_{k+1}) + D_k^{22} - D_k^{21}(J^F(\Theta_k) + D_k^{11})^{-1} D_k^{12} \\ &= \frac{1}{\sigma_0^2} + \frac{1}{\sigma_\phi^2} - \frac{1}{\sigma_\phi^4}\left(J^F(\Theta_k) + \frac{1}{\sigma_\phi^2}\right)^{-1} \triangleq \tilde{J}^F(\Theta_{k+1}) + \frac{1}{\sigma_0^2} \\ J^B(\Theta_k) &= J^U(\Theta_k) + D_k^{11} - D_k^{12}(J^B(\Theta_{k+1}) + D_k^{11})^{-1} D_k^{21} \\ &= \frac{1}{\sigma_0^2} + \frac{1}{\sigma_\phi^2} - \frac{1}{\sigma_\phi^4}\left(J^B(\Theta_{k+1}) + \frac{1}{\sigma_\phi^2}\right)^{-1} \triangleq \tilde{J}^B(\Theta_{k+1}) + \frac{1}{\sigma_0^2}. \end{aligned}$$

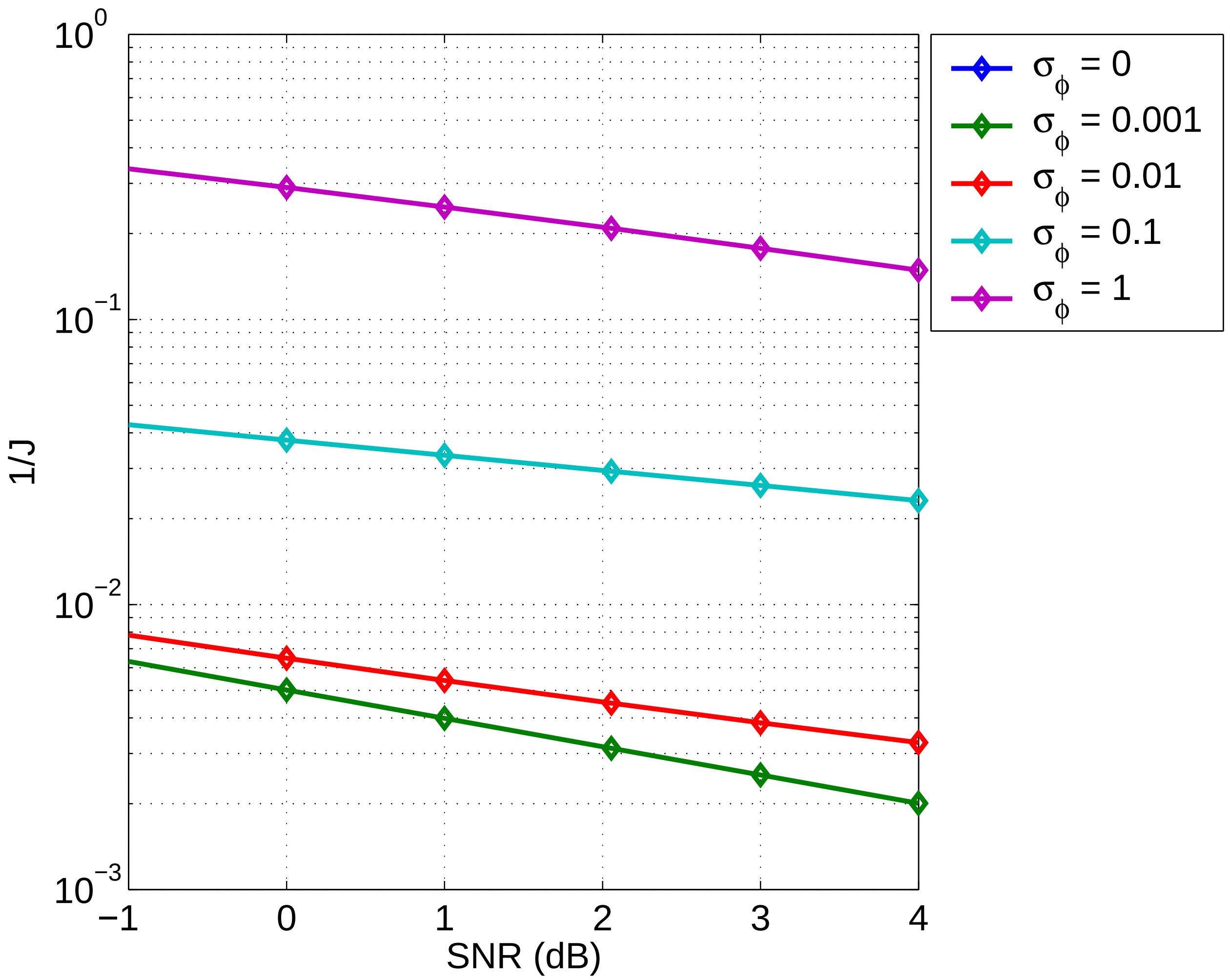
Example 1 (4)

Random walk phase model $(N = 100, \sigma_0^2 = 0.1991, \sigma_\phi^2 = 0.01)$



Example 1 (5)

Random walk phase model

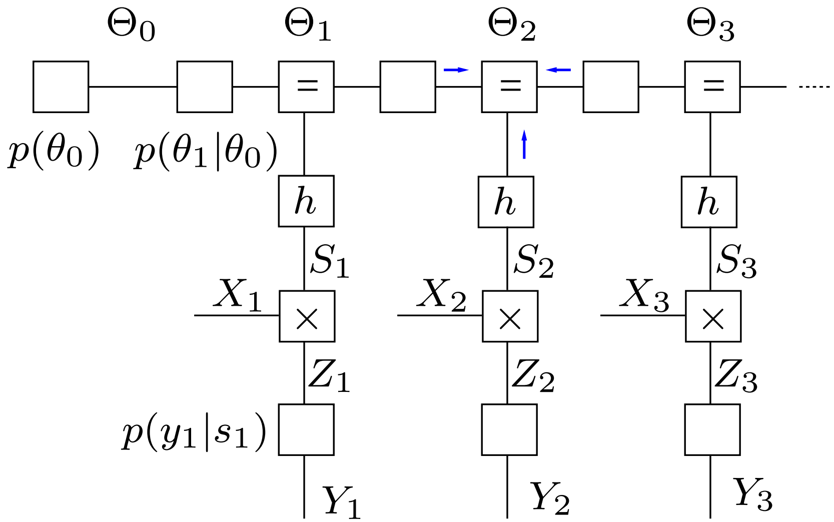


Example 2

Code + Random walk phase model

$$\begin{aligned} \Theta_{k+1} &= (\Theta_k + W_k) \bmod 2\pi \\ Y_k &= X_k \exp(j\Theta_k) + V_k, \end{aligned}$$

where W_k and V_k are i.i.d. (mean free) Gaussian RVs with variance σ_θ^2 and $2\sigma_0^2$ resp. and X_k are M-ary symbols protected by an error correcting code.



$S_i \triangleq \exp(j\Theta_i)$

$h(\theta_k, s_k) \triangleq \delta(s_k - \exp(j\theta_k))$

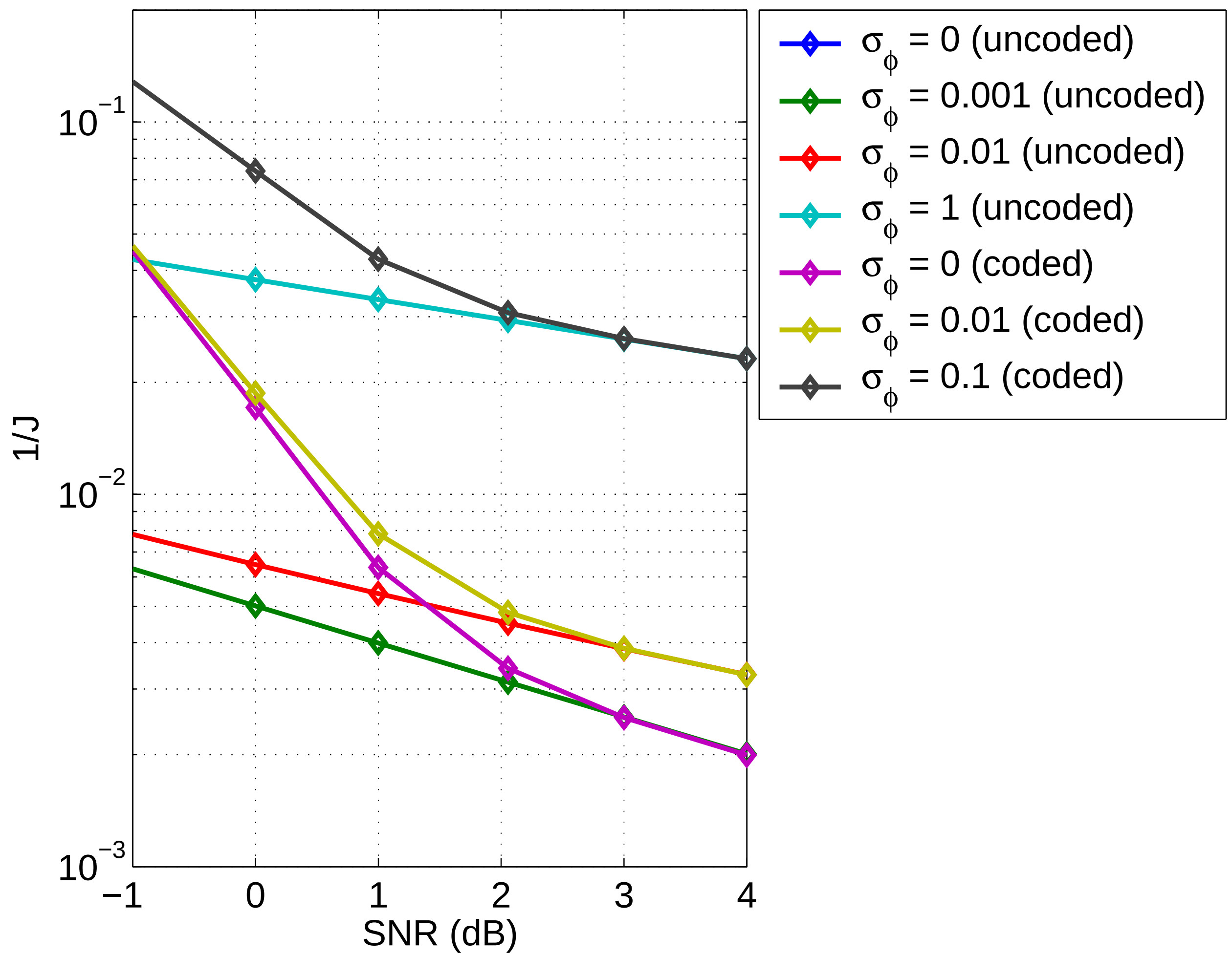
$p(y_k|s_k) \triangleq (2\pi\sigma_N^2)^{-1} \, \exp(-||y_k - s_k||^2/2\sigma_N^2)$

$p(\theta_k|\theta_{k-1}) \triangleq (2\pi\sigma_W^2)^{-1/2} \, \sum_{n\in\mathbb{Z}} \exp(-((\theta_k - \theta_{k-1}) + n2\pi)^2/2\sigma_W^2)$

$h_\times(s_k, z_k) = \delta(z_k - x_k s_k)$.

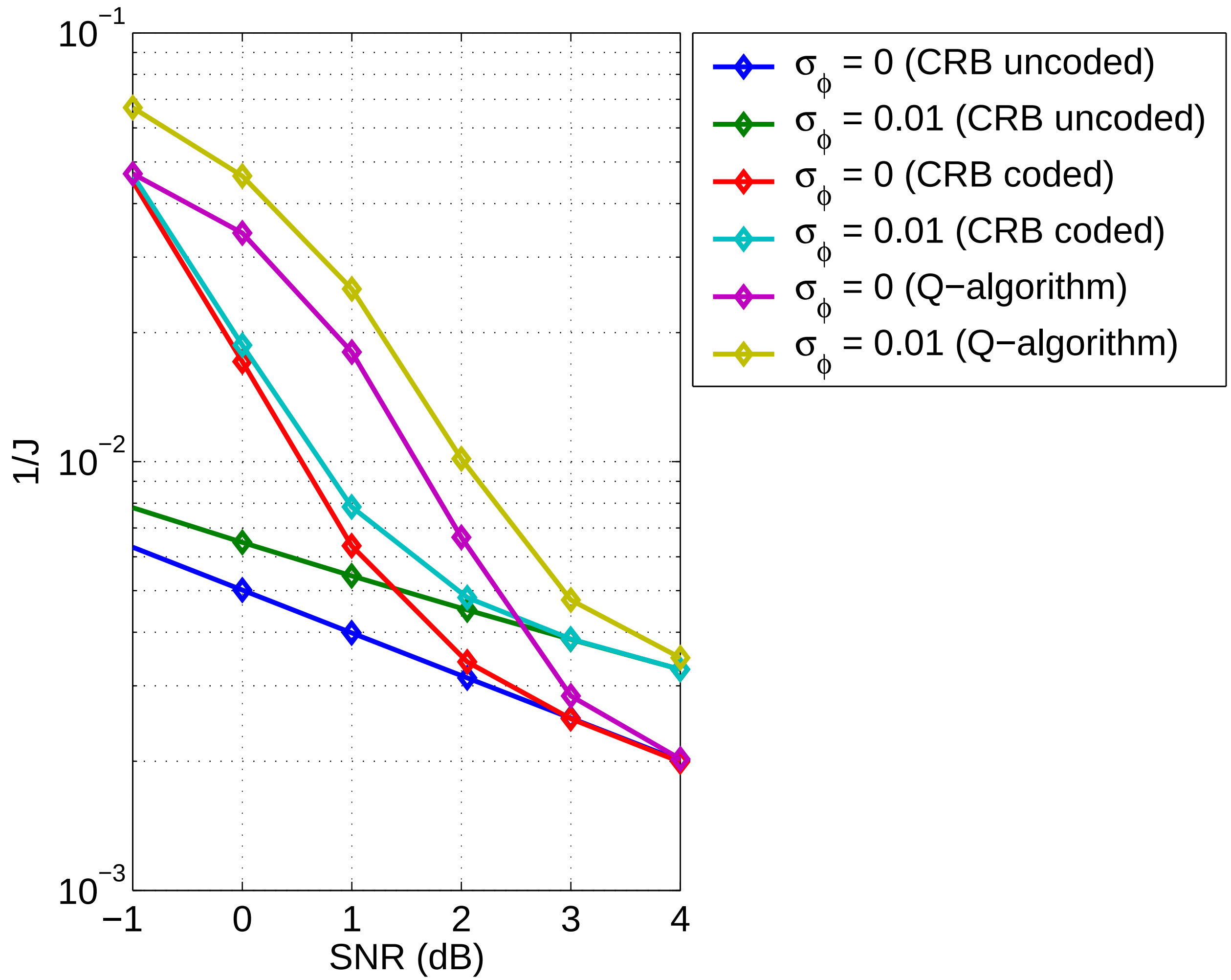
Example 2 (2)

Code + Random walk phase model (3-6 LDPC of length 100)



Example 2 (3)

Code + Random walk phase model (3-6 LDPC of length 100)



Conclusion

- CRBs have previously been computed for
  - parameter estimation
  - filtering (of states).
- We extended this to
  - estimation on trees
    e.g., filtering and smoothing of input and/or state.
  - estimation on certain cyclic graphs, i.e., code + channel.
    e.g., code + random walk phase model.

Thank you for your attention!

Computing Cramér-Rao bounds in graphical models

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