

Expectation Maximization as Message Passing—Part I: Principles and Gaussian Messages

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Abstract—It is shown how expectation maximization (EM) may be viewed as a message passing algorithm in factor graphs. In particular, a general EM message computation rule is identified. As a factor graph tool, EM may be used to break cycles in a factor graph, and tractable messages may in some cases be obtained where the sum-product messages are unwieldy.

As an exemplary application, the paper considers linear Gaussian state space models. Unknown coefficients in such models give rise to multipliers in the corresponding factor graph. A main attraction of EM in such cases is that it results in purely Gaussian message passing algorithms. These Gaussian EM messages are tabulated for several (scalar, vector, matrix) multipliers that frequently appear in applications.

Index Terms—Expectation maximization, factor graphs, message passing.

I. INTRODUCTION

Graphical models [1] in general and factor graphs [2]–[5] in particular provide a notation for structured system models that helps to describe and to develop algorithms for detection and estimation problems. A large variety of algorithms can be viewed as message passing algorithms that operate by passing locally computed “messages” along the edges of the factor graph.

Expectation maximization (EM) [6]–[9] is an iterative technique for parameter estimation which is widely used in statistics and signal processing. EM is a standard tool for parameter estimation in graphical models [10], [11], but EM has not traditionally been viewed as a message passing algorithm. Examples in communications include turbo synchronization [12]–[14], joint channel estimation and symbol detection [15]–[17], and distributed source coding [18].

An explicit formulation of a “factor graph EM algorithm” was proposed in [19] and [20], and a full description of EM

as a message passing algorithm with a general local message computation rule was presented in [21], which is the basis of the present paper. A similar approach was also pursued by O’Sullivan [22] and by Herzet et al. [14].

In a parallel development, Winn and Bishop made the important observation that variational inference can be put into message passing form [23], [24], and similar observations were made also in [25] and [26]. In fact, EM message passing may be viewed as a special case of variational message passing [27]. However, EM is not specifically addressed (and not even mentioned) in [23]–[25].

In this paper and its companion paper [28], we develop the EM algorithm as a general message passing technique for factor graphs. This formulation may be helpful in several different ways:

- EM may be used to estimate unknown parameters in a factor graph model.
- EM may be used to break cycles in a factor graph.
- The EM messages are tractable expressions in some cases where the sum-product and max-product message computation rules yields intractable expressions.
- Tabulated EM messages for frequently occurring nodes/factors allow the composition of nontrivial EM algorithms without additional computations or derivations.

Conversely, the flexibility of the factor graph approach suggests many variations and extensions of the EM algorithm itself, as will be discussed in Section VI and in [28]. Moreover, the EM message passing algorithm may be seamlessly combined with sum-product and max-product message passing in various ways.

This paper begins with a brief review of standard EM in Section II and a detailed development of message passing EM in Section III. As quite some time has passed since the publication of [19]–[21], this part of the paper is perhaps mainly tutorial.

In Section IV, we illustrate message passing EM by its application to linear Gaussian models (in particular, FIR filters and autoregressive filters) with unknown coefficients. In these examples, the EM messages turn out to be Gaussian, which yields a fully Gaussian algorithm for these nonlinear problems.

These examples also illustrate the use of tabulated EM message computation rules. The derivation of the EM message

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Some parts of this work were presented in preliminary form in [19], [20], [21].

for a particular application is often not trivial and tables of precomputed EM messages can therefore be helpful. In Section V, we present tables of EM messages out of various “multipliers” that arise naturally in linear Gaussian models with unknown coefficients.

The proofs of these tabulated message computation rules are given in Appendices C–E. Appendices D and E rely on Gaussian sum-product messages tabulated in [5], which further illustrates the use of tabulated message computation rules.

Some concluding remarks are offered in Section VI.

The companion paper [28] begins with discrete variables and makes a tour through EM algorithms ranging from hidden Markov models to independent factor analysis.

In this paper, we will use Forney-style factor graphs (also called normal factor graphs) as in [4] and [5], a variation due to Forney [29] of factor graphs as in [3]. The reader is specifically referred to [5] for details of the factor graph notation. In particular, we will use arrows (as in $\vec{\mu}$ and $\overleftarrow{\mu}$) for sum-product messages, and we will use capital letters for unknown variables (i.e., functions of the configuration space) and lower-case letters for particular values of a variable.

From Section IV onward, multivariate Gaussian distributions will be prominent. Such distributions will be parameterized either by a mean vector m and a covariance matrix V or by the inverse covariance matrix (“weight matrix”) $W = V^{-1}$ and the transformed mean vector Wm . For Gaussian messages, these parameters will be denoted by \vec{m} , \vec{V} , etc., as in [5]. We will sometimes allow messages to be degenerate (non-integrable) “Gaussians” $e^{-\frac{1}{2}(x^T W x - 2x^T W m)}$ where the weight matrix W is positive semi-definite and singular rather than positive definite.

II. REVIEW OF THE EM ALGORITHM

We begin by reviewing the EM algorithm in a setting which is suitable for the purpose of this paper. Suppose we wish to find

$$\hat{\theta}_{\max} \triangleq \operatorname{argmax}_{\theta} f(\theta) \quad (1)$$

for some function $f : \mathbb{R}^n \rightarrow \mathbb{R}$. We assume that $f(\theta)$ is the “marginal” of some real-valued function $f(x, \theta)$, i.e.,

$$f(\theta) = \int_x f(x, \theta) dx \quad (2)$$

where $\int_x g(x) dx$ denotes integration of $g(x)$ over the whole range of x . (The integral in (2) may be replaced by a sum if x is discrete, with obvious corresponding changes in subsequent expressions.) The function $f(x, \theta)$ is assumed to be nonnegative:

$$f(x, \theta) \geq 0 \quad \text{for all } x \text{ and all } \theta. \quad (3)$$

In addition, we assume $0 < f(\theta) < \infty$ for all θ . In other words, for any fixed θ , $f(x, \theta)/f(\theta)$ is a probability density over x . We will also assume that the integral $\int_x f(x, \theta) \log f(x, \theta') dx$ exists for all θ, θ' .

The EM algorithm attempts to compute (1) as follows:

- 1) Make some initial guess $\hat{\theta}^{(0)}$.

- 2) Expectation step: evaluate

$$f^{(k)}(\theta) \triangleq \int_x f(x, \hat{\theta}^{(k)}) \log f(x, \theta) dx. \quad (4)$$

(The base of the logarithm is immaterial.)

- 3) Maximization step: compute

$$\hat{\theta}^{(k+1)} \triangleq \operatorname{argmax}_{\theta} f^{(k)}(\theta). \quad (5)$$

- 4) Repeat 2–3 until convergence or until the available time is over.

The main property of the EM algorithm is

$$f(\hat{\theta}^{(k+1)}) \geq f(\hat{\theta}^{(k)}). \quad (6)$$

For the reader’s convenience, a concise proof of (6) is given in Appendix A. In many applications, the expressions (4) and (5) turn out to be quite manageable and simpler than the direct maximization (1).

In typical applications, $f(x, \theta)$ is extended to $f(x, y, \theta)$, where y is known and fixed. The function $f(x, y, \theta)$ is either a probability density over x and y with parameter θ or it is a joint probability density over x , y , and θ . In the EM literature, y is called the observed data, x is called the missing (unobserved) data, and the pair (x, y) is called the complete data.

III. EM AS A MESSAGE PASSING ALGORITHM

We now consider EM in factor graphs. We will do this in several steps. The resulting message passing algorithm will be summarized in Section III-E.

We henceforth assume that all logarithms are natural logarithms.

A. Trivial Factor Graph

We first consider a trivial factorization

$$f(x, \theta) = f_A(\theta) f_B(x, \theta), \quad (7)$$

the factor graph of which is shown in Fig. 1. (In typical applications, $f_A(\theta)$ is either a prior probability or constant.) In this setup, the EM algorithm amounts to iterative computation of a downward message $\hat{\theta}^{(k)}$ and an upward message $e^{\eta(\theta)}$ as follows.

Upward message (EM message): $e^{\eta(\theta)}$ with

$$\eta(\theta) \triangleq \frac{\int_x f_B(x, \hat{\theta}^{(k)}) \log f_B(x, \theta) dx}{\int_x f_B(x, \hat{\theta}^{(k)}) dx} \quad (8)$$

$$= E_{p_B}[\log f_B(X, \theta)], \quad (9)$$

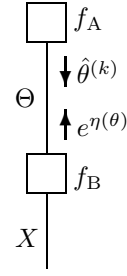


Fig. 1. Factor graph of (7) with EM message $e^{\eta(\theta)}$.

where E_{p_B} denotes the expectation with respect to the probability distribution

$$p_B(x|\hat{\theta}^{(k)}) \triangleq \frac{f_B(x, \hat{\theta}^{(k)})}{\int_{x'} f_B(x', \hat{\theta}^{(k)}) dx'} \quad (10)$$

Downward message:

$$\hat{\theta}^{(k+1)} = \operatorname{argmax}_{\theta} \left(f_A(\theta) \cdot e^{\eta(\theta)} \right) \quad (11)$$

$$= \operatorname{argmax}_{\theta} (\log f_A(\theta) + \eta(\theta)). \quad (12)$$

The equivalence of this message passing algorithm with (4) and (5) may be seen as follows. From (4) and (5), we have

$$\hat{\theta}^{(k+1)} = \operatorname{argmax}_{\theta} \int_x f(x, \hat{\theta}^{(k)}) \log f(x, \theta) dx \quad (13)$$

$$= \operatorname{argmax}_{\theta} \int_x f_A(\hat{\theta}^{(k)}) f_B(x, \hat{\theta}^{(k)}) \cdot \log(f_A(\theta) f_B(x, \theta)) dx \quad (14)$$

$$= \operatorname{argmax}_{\theta} \int_x f_B(x, \hat{\theta}^{(k)}) \cdot \left(\log f_A(\theta) + \log f_B(x, \theta) \right) dx \quad (15)$$

$$= \operatorname{argmax}_{\theta} \left(\log f_A(\theta) + \frac{\int_x f_B(x, \hat{\theta}^{(k)}) \log f_B(x, \theta) dx}{\int_{x'} f_B(x', \hat{\theta}^{(k)}) dx'} \right) \quad (16)$$

which is equivalent to (8) and (12).

Some remarks:

- 1) The quantity $\eta(\theta)$ may be viewed as a ‘‘log-domain’’ summary of f_B . The corresponding ‘‘probability domain’’ summary $e^{\eta(\theta)}$ is consistent with the semantics of factor graphs where messages are ‘‘summaries’’ of factors (cf. (11) and (22)). We will refer to $e^{\eta(\theta)}$ as the *EM message*.
- 2) A constant may be added to $\eta(\theta)$ without affecting (12).
- 3) If $f_A(\theta)$ is constant, the normalization in (8) can be omitted. More generally, the normalization in (8) can be omitted if $f_A(\theta)$ is constant for all θ such that $f_A(\theta) \neq 0$ (i.e., if $f_A(\theta)$ expresses a constraint); this case occurs in many applications.
- 4) Nothing changes if we introduce a known observation (i.e., a constant argument) y into f such that (7) becomes $f(x, y, \theta) = f_A(y, \theta) f_B(x, y, \theta)$.

B. Nontrivial Factor Graph

We now come to the heart of the matter: if θ is a vector, $\theta = (\theta_1, \theta_2, \dots)$, and if f_B has a nontrivial factor graph, then the EM message $e^{\eta(\theta)}$ splits into messages $e^{\eta_1(\theta_1)}, e^{\eta_2(\theta_2)}, \dots$ that can be computed ‘‘locally’’ in the factor graph of f_B .

To see this, consider the following example (which actually covers the general case). Let $\theta = (\theta_1, \theta_2)$, let $x = (x_1, x_2, x_3)$, and let

$$f_B(x, \theta) = f_C(x_1, x_2, \theta_1) f_D(x_2, x_3, \theta_2), \quad (17)$$

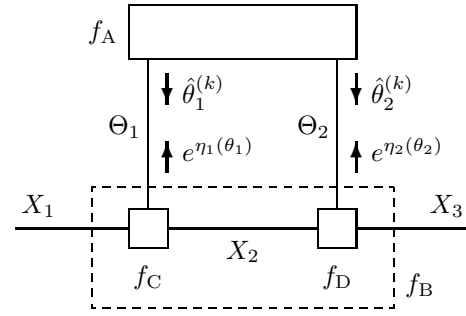


Fig. 2. Factor graph of (17), a refinement of Fig. 1.

the factor graph of which is shown in Fig. 2. In this case, (9) splits into

$$\eta(\theta_1, \theta_2) = E_{p_B} \left[\log \left(f_C(X_1, X_2, \theta_1) f_D(X_2, X_3, \theta_2) \right) \right] \quad (18)$$

$$= \eta_1(\theta_1) + \eta_2(\theta_2) \quad (19)$$

with

$$\eta_1(\theta_1) \triangleq E_{p_B} [\log f_C(X_1, X_2, \theta_1)] \quad (20)$$

and

$$\eta_2(\theta_2) \triangleq E_{p_B} [\log f_D(X_2, X_3, \theta_2)]. \quad (21)$$

The EM message $e^{\eta(\theta)}$ thus factors as

$$e^{\eta(\theta_1, \theta_2)} = e^{\eta_1(\theta_1)} e^{\eta_2(\theta_2)}, \quad (22)$$

and the factors $e^{\eta_1(\theta_1)}$ and $e^{\eta_2(\theta_2)}$ may be viewed as upward messages along the edge Θ_1 and Θ_2 , respectively, in the factor graph of Fig. 2. The downward messages in Fig. 2 are the estimates

$$(\hat{\theta}_1^{(k+1)}, \hat{\theta}_2^{(k+1)}) = \operatorname{argmax}_{(\theta_1, \theta_2)} f_A(\theta_1, \theta_2) e^{\eta_1(\theta_1)} e^{\eta_2(\theta_2)} \quad (23)$$

as is obvious from (11) and (22).

The expectation in (20) may be computed with respect to the probability distribution

$$p_B(x_1, x_2 | \hat{\theta}^{(k)}) \triangleq \int_{x_3} p_B(x_1, x_2, x_3 | \hat{\theta}^{(k)}) dx_3, \quad (24)$$

which is the marginal of p_B with respect to the arguments of f_C , and the expectation in (21) may be computed with respect to the probability distribution

$$p_B(x_2, x_3 | \hat{\theta}^{(k)}) \triangleq \int_{x_1} p_B(x_1, x_2, x_3 | \hat{\theta}^{(k)}) dx_1, \quad (25)$$

which is the marginal of p_B with respect to the arguments of f_D .

Going through this derivation, we note that the generalization to an arbitrary factor graph for f_B is immediate. Note, in particular, that the splitting of the expectation in (19) does not assume that the factor graph of f_B is cycle-free. If $g(x_1, \dots, x_m, \theta_g)$ is a generic node / factor in the factor graph of f_B , we obtain $\eta_g(\theta_g)$ as in (I.1) and (I.2) in Table I with

$$p_{\text{local}}(x_1, \dots, x_m | \hat{\theta}) \triangleq \int_{x: x_1 \dots x_m \text{ fixed}} p_B(x | \hat{\theta}) dx \quad (26)$$

$$\propto \int_{x: x_1 \dots x_m \text{ fixed}} f_B(x, \hat{\theta}) dx, \quad (27)$$

TABLE I
EM MESSAGE $e^{\eta_g(\theta_g)}$ OUT OF A GENERIC NODE / FACTOR g .

$\eta_g(\theta_g) = \mathbb{E}_{p_{\text{local}}} [\log g(X_1, \dots, X_m, \theta_g)] \quad (\text{I.1})$
$= \int_{x_1, \dots, x_m} p_{\text{local}}(x_1, \dots, x_m \hat{\theta}) \cdot \log g(x_1, \dots, x_m, \theta_g) dx_1 \cdots dx_m \quad (\text{I.2})$
with
$p_{\text{local}}(x_1, \dots, x_m \hat{\theta}) \propto g(x_1, \dots, x_m, \hat{\theta}) \vec{\mu}_{X_1}(x_1) \cdots \vec{\mu}_{X_m}(x_m) \quad (\text{I.3})$
where $\vec{\mu}_{X_\ell}$ denotes the incoming sum-product message along the variable / edge X_ℓ computed for $\Theta = \hat{\theta}$.
A constant scale factor γ in g results in a scale factor γ in $e^{\eta_g(\theta_g)}$ which can be ignored.

where “ \propto ” denotes equality up to a scale factor. Note that the missing scale factor in (27) can be locally recovered by integrating (27) over $x_1 \dots x_m$. It remains to make the step from (27) to (I.3) in Table I.

C. Using Sum-Product Message Passing for the Local Expectations

If the factor graph of $f_B(x, \hat{\theta})$ is cycle-free (after removing the edges for $\Theta = \hat{\theta}$), then the marginals (27) can be computed by sum-product message passing (see [4], [5]) in this factor graph. As above, let $g(x_1, \dots, x_m, \theta_g)$ be a generic node/factor in the factor graph of f_B . Then (27) may be computed as in (I.3) in Table I, where $\vec{\mu}_{X_\ell}$ denotes the incoming sum-product message along the variable/edge X_ℓ computed for $\Theta = \hat{\theta}$.

For example, we can write (24) as

$$p_B(x_1, x_2 | \hat{\theta}) \propto \int_{x_3} f_C(x_1, x_2, \hat{\theta}_1) f_D(x_2, x_3, \hat{\theta}_2) dx_3 \quad (28)$$

$$= f_C(x_1, x_2, \hat{\theta}_1) \overleftarrow{\mu}_{X_2}(x_2) \quad (29)$$

where $\overleftarrow{\mu}_{X_2}$ is the right-to-left sum-product message along the edge X_2 computed for $\Theta = \hat{\theta}$. (A constant message $\overleftarrow{\mu}_{X_1}(x_1) = 1$ may be added as a factor in (29).)

D. Using Max-Product Message Passing for the Maximization

If f_A can be factored into a cycle-free factor graph, then the maximization (23) (and its obvious generalization to general factor graphs) can be carried out by max-product message

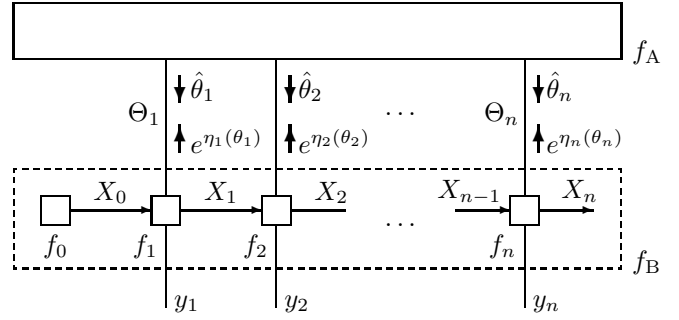


Fig. 3. Application of EM to general state space model.

passing in the factor graph of f_A . This applies, in particular, to the standard case where $f_A(\theta_1, \theta_2, \dots)$ expresses the equality constraint $\Theta_1 = \Theta_1 = \dots$, which we will encounter in Section IV.

E. Putting it Together

Let us summarize the findings of this section by considering the factor graph of Fig. 3, which is an easy generalization of Fig. 2. Note that removing the edges $\Theta_1, \dots, \Theta_n$ cuts the factor graph (Fig. 3) into two cycle-free components. Let $\theta \triangleq (\theta_1, \dots, \theta_n)$, $x \triangleq (x_1, \dots, x_n)$, and $y \triangleq (y_1, \dots, y_n)$. Suppose that we wish to find

$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}} f_A(\theta) \int_x f_B(x, y, \theta) dx \quad (30)$$

for fixed known y . In this case, the EM algorithm applies as follows:

- 1) Make some initial guess $\hat{\theta} = (\hat{\theta}_1, \dots, \hat{\theta}_n)$.
- 2) Perform forward-backward sum-product message passing through the factor graph of f_B (with $\hat{\theta}_\ell$ plugged into f_ℓ for $\ell = 1, \dots, n$).
- 3) Compute the EM messages $e^{\eta_1(\theta_1)}, \dots, e^{\eta_n(\theta_n)}$ as in Table I. In this case, we obtain

$$\eta_\ell(\theta_\ell) = \mathbb{E}_{p_{\text{local}}} [\log f_\ell(X_{\ell-1}, X_\ell, y_\ell, \theta_\ell)] \quad (31)$$

where the expectation is with respect to the probability density

$$p_{\text{local}}(x_{\ell-1}, x_\ell | y_\ell, \hat{\theta}) \propto f_\ell(x_{\ell-1}, x_\ell, y_\ell, \hat{\theta}_\ell) \cdot \vec{\mu}_{X_{\ell-1}}(x_{\ell-1}) \overleftarrow{\mu}_{X_\ell}(x_\ell) \quad (32)$$

where $\vec{\mu}_{X_{\ell-1}}$ and $\overleftarrow{\mu}_{X_\ell}$ denote sum-product messages.

- 4) Compute new estimates

$$\hat{\theta} = (\hat{\theta}_1, \dots, \hat{\theta}_n) \quad (33)$$

$$= \underset{(\theta_1, \dots, \theta_n)}{\operatorname{argmax}} f_A(\theta_1, \dots, \theta_n) e^{\eta_1(\theta_1)} \cdots e^{\eta_n(\theta_n)}. \quad (34)$$

If f_A has a cycle-free factor graph, this maximization may be carried out by max-product message passing in that factor graph.

- 5) Repeat 2–4 until convergence or until the available time is over.

All this applies to general factorizations of f_A and f_B provided that the resulting factor graphs (without the edges $\Theta_1, \dots, \Theta_n$) are cycle-free.

If the factor graphs of f_A and f_B are not cycle-free, the same local computation rules can be used nonetheless and seem to work well in some applications, cf. [12]–[18].

In many cases, the computation of an EM message according to Table I requires substantial additional work. Pre-computed tables of such messages for frequently occurring nodes/factors can therefore be useful, as will be demonstrated in Sections IV and V.

F. An Issue: Hard Constraints and Grouping

Nodes in factor graphs often express “hard” constraints [4], [5]. For example, the constraint $X_1 = X_2$ (for real variables X_1 and X_2) may be expressed by the node/factor $\delta(x_1 - x_2)$, where δ denotes the Dirac delta. It turns out that the EM message computation rule of Table I should not be applied to such constraint nodes; the typical outcome of the attempt will be a degenerate EM message $e^{\eta_s(\theta_s)}$ that expresses the constraint $\Theta_s = \hat{\theta}_s$, which stalls the EM algorithm.

For example, assume that X_1, X_2, Θ are real variables and the node/factor

$$g(x_1, x_2, \theta) = \delta(x_1 - x_2\theta) \quad (35)$$

expresses the constraint $X_1 = X_2\theta$. Then

$$\eta(\theta) \propto \int_{x_1} \int_{x_2} g(x_1, x_2, \hat{\theta}) \vec{\mu}_{X_1}(x_1) \vec{\mu}_{X_2}(x_2) \cdot \log g(x_1, x_2, \theta) dx_1 dx_2 \quad (36)$$

$$= \int_{x_2} \vec{\mu}_{X_1}(x_2\hat{\theta}) \vec{\mu}_{X_2}(x_2) \log g(x_2\hat{\theta}, x_2, \theta) dx_2 \quad (37)$$

$$= \int_{x_2} \vec{\mu}_{X_1}(x_2\hat{\theta}) \vec{\mu}_{X_2}(x_2) \log \delta(x_2(\hat{\theta} - \theta)) dx_2, \quad (38)$$

which is obviously pathological and illustrates the issue.

It is usually easy to avoid this problem by grouping constraint nodes with adjacent “soft” factors/nodes, as will be illustrated in Sections IV and V.

IV. EXAMPLES: IDENTIFICATION OF LINEAR SYSTEMS

The following two examples arise in many applications. The use of EM to problems of this kind is not new, but neither is it trivial [33]–[35]. In communications, the example of Section IV-A may arise in channel estimation and the example of Section IV-B may arise in estimating the parameters of non-white Gaussian noise.

A. FIR Filter Identification with Unknown Input Signal

Let $X_k \in \mathbb{R}^n$, $k = 0, 1, 2, \dots, N$, be the time- k state of a finite impulse response (FIR) filter with random input signal $U_k \in \mathbb{R}$, $k = 1, 2, \dots, N$. Specifically,

$$X_k = AX_{k-1} + bU_k \quad (39)$$

with $n \times n$ matrix

$$A = \begin{pmatrix} 0 & 0 \\ I_{n-1} & 0 \end{pmatrix} \quad (40)$$

(where I_{n-1} is the $(n-1) \times (n-1)$ identity matrix) and with

$$b = (1, 0, \dots, 0)^T. \quad (41)$$

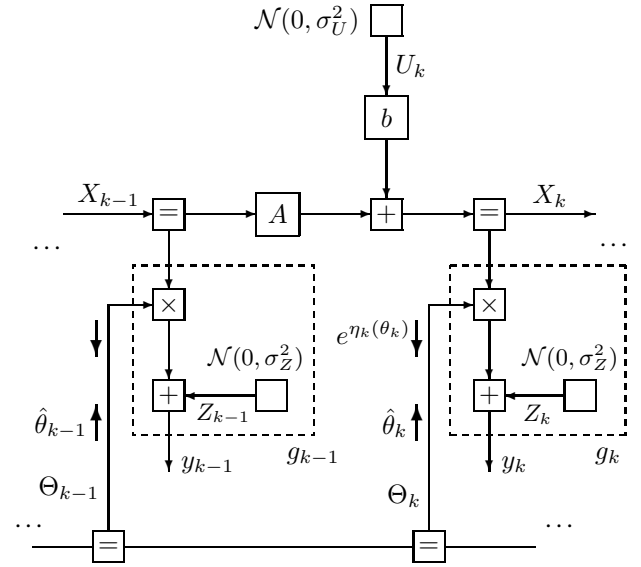


Fig. 4. Linear state space model with unknown coefficient vector $\Theta = \Theta_1 = \Theta_2 = \dots$ and white Gaussian input signal U_1, U_2, \dots . The figure shows one section of the factor graph. The multiplier node denotes the inner product $\Theta_k^T X_k$. The label $\mathcal{N}(m, \sigma^2)$ denotes a scalar Gaussian factor with mean m and variance σ^2 . The EM message computation rule is applied to the dashed boxes.

We assume that the input signal U_1, U_2, \dots is zero-mean white Gaussian noise with variance σ_U^2 . We observe a noisy scalar output signal

$$Y_k = \Theta^T X_k + Z_k \quad (42)$$

where Θ is an unknown real column vector and where Z_k is zero-mean white Gaussian noise with variance σ_Z^2 . From the observations $Y_k = y_k$, $k = 1, 2, \dots, N$, we wish to estimate Θ . Specifically, we wish to compute the maximum-likelihood estimate

$$\hat{\theta} = \operatorname{argmax}_{\theta} p(y|\theta) \quad (43)$$

$$= \operatorname{argmax}_{\theta} \int_u \int_x \int_z p(u, x, y, z|\theta) dz dx du, \quad (44)$$

where y is defined as $y \triangleq (y_1, \dots, y_N)$ and where u, x, z are defined analogously.

The factor graph of this system model, i.e., of

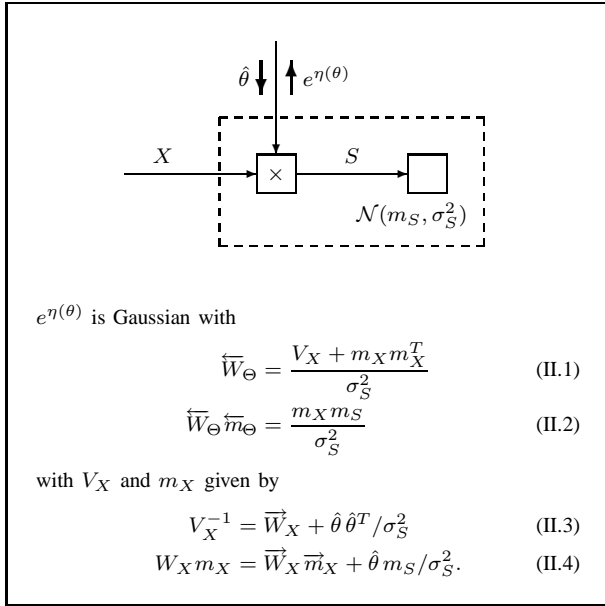
$$p(u, x, y, z|\theta) = p(x_0) \prod_{k=1}^N p(y_k|x_k, z_k, \theta) p(z_k) p(x_k|x_{k-1}, u_k) p(u_k), \quad (45)$$

is shown in Fig. 4. Note that the unknown coefficient vector Θ appears in copies Θ_k , $k = 1, 2, \dots, N$ (one copy for each time k) with an equality constraint $\Theta_1 = \dots = \Theta_N$. Note also that the factors $p(x_k|x_{k-1}, u_k)$ and $p(y_k|x_k, z_k, \theta)$ express the constraints (39) and (42), respectively; only the scalar Gaussian factors $p(u_k)$ and $p(z_k)$ are “soft” factors without Dirac deltas. The factor $p(x_0)$ (not shown in Fig. 4) is of secondary importance and may even be omitted in practice.

Note that the edges Θ_k , $k = 1, 2, \dots$, cut the factor graph into two cycle-free components. The equality constraints $\Theta_1 =$

TABLE II

GAUSSIAN MESSAGE PASSING BACKWARDS THROUGH A MULTIPLIER. X AND Θ ARE REAL COLUMN VECTORS AND $S = \Theta^T X$ IS A SCALAR. $\mathcal{N}(m, \sigma^2)$ DENOTES A SCALAR GAUSSIAN FACTOR WITH MEAN m AND VARIANCE σ^2 . THE INCOMING SUM-PRODUCT MESSAGE $\overrightarrow{\mu}_X$ IS GAUSSIAN WITH PARAMETERS \overrightarrow{W}_X AND \overrightarrow{m}_X .



$\Theta_2 = \dots$ at the bottom of Fig. 4 correspond to f_A in Figures 2 and 3; everything else in Fig. 4 corresponds to f_B in Figures 2 and 3.

With estimates $\hat{\theta}_k$ plugged in, the upper part (the f_B part) of Fig. 4 becomes a standard linear Gaussian factor graph, where sum-product message passing amounts to Kalman filtering/smoothing [5, Section V].

We now need to compute the EM messages $e^{\eta_k(\theta_k)}$. Heeding the advice of Section III-F, we group the multiplier node (which is a hard constraint) with the adjacent soft node/factor $p(z_k) \propto e^{-z_k^2/(2\sigma_Z^2)}$ as indicated by the dashed boxes in Fig. 4; this grouping (and integrating/marginalizing over the variables inside the box) results in the factor

$$g_k(x_k, y_k, \theta_k) = \int_{z_k} \delta(\theta_k^T x_k + z_k - y_k) \frac{1}{\sqrt{2\pi\sigma_Z^2}} e^{-z_k^2/(2\sigma_Z^2)} dz_k \quad (46)$$

$$\propto e^{-(\theta_k^T x_k - y_k)^2/(2\sigma_Z^2)}, \quad (47)$$

which is perfectly well-behaved. Note that the missing scale factor in (47) can be safely ignored, cf. Table I.

As it turns out, the EM message $e^{\eta_k(\theta_k)}$ out of the dashed box g_k in Fig. 4 is Gaussian with weight matrix (inverse covariance matrix) $\overleftarrow{W}_{\Theta_k}$ and mean vector $\overleftarrow{m}_{\Theta_k}$ as given by (II.1)-(II.4) in Table II with $m_S = y_k$ and $\sigma_S^2 = \sigma_Z^2$. The proof of (II.1)-(II.4) is given in Section V.

It remains only to compute new estimates $\hat{\theta}_k$ by max-product message passing through the chain of equality constraints at the bottom of Fig. 4. Since the incoming EM messages $e^{\eta_k(\theta_k)}$ are Gaussians, max-product message passing coincides with sum-product message passing with message computation rules as in Table 2 of [5].

In summary, both the expectation step and the maximization step of the EM algorithm can be carried out by Gaussian message passing.

B. Autoregressive Filter Identification

Consider the following state space representation of an autoregressive model. Let the state $X_k \in \mathbb{R}^n$, $k = 1, 2, \dots, N$ evolve according to

$$X_k = AX_{k-1} + bU_k \quad (48)$$

with

$$b = (1, 0, \dots, 0)^T \quad (49)$$

and with $n \times n$ matrix

$$A(\Theta) = \begin{pmatrix} \Theta^T & \\ I_{n-1} & 0 \end{pmatrix} \quad (50)$$

where Θ is an unknown column vector of dimension n . We assume that the input signal U_1, U_2, \dots , which is often called ‘‘innovation’’, is zero-mean white Gaussian noise with variance σ_U^2 . We observe a noisy scalar output signal

$$Y_k = (1, 0, \dots, 0)^T X_k + Z_k, \quad (51)$$

where Z_1, Z_2, \dots is zero-mean white Gaussian noise with variance σ_Z^2 . From the observation $Y_k = y_k$, $k = 1, 2, \dots, N$, we wish to estimate Θ ; specifically, we wish to compute the maximum likelihood estimate

$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}} p(y|\theta) \quad (52)$$

$$= \underset{\theta}{\operatorname{argmax}} \int_u \int_x \int_z p(u, x, y, z|\theta) dz dx du \quad (53)$$

with $y \triangleq (y_1, y_2, \dots, y_N)$ etc.

The factor graph of $p(u, x, y, z|\theta)$ is shown in Fig. 5. As in the previous example, the unknown parameter vector Θ appears in copies $\Theta_1 = \dots = \Theta_N$, one copy for each time k .

Again, for fixed $\Theta = \hat{\theta}$, this factor graph is linear Gaussian and cycle-free.

The EM message computation rule of Table I may be applied to the dashed box in Fig. 5. It turns out that the EM message $e^{\eta_k(\theta_k)}$ is Gaussian with mean $\overleftarrow{m}_{\Theta_k}$ and weight matrix (inverse covariance matrix) $\overleftarrow{W}_{\Theta_k}$ given by (III.7) and (III.8) in Table III.

Again, we have obtained a purely Gaussian message passing algorithm. Apart from the EM message $e^{\eta_k(\theta_k)}$, all messages can be computed as described in [5, Section V].

C. Remarks

We conclude this section with some remarks on these examples.

- 1) In order to make the described algorithms work in practice, it is necessary to pay attention to the scheduling of the message updates. A serial (left-to-right) schedule may actually work better than alternating forward-backward sweeps in the two components (corresponding to f_A and f_B) of the factor graph, cf. [30].

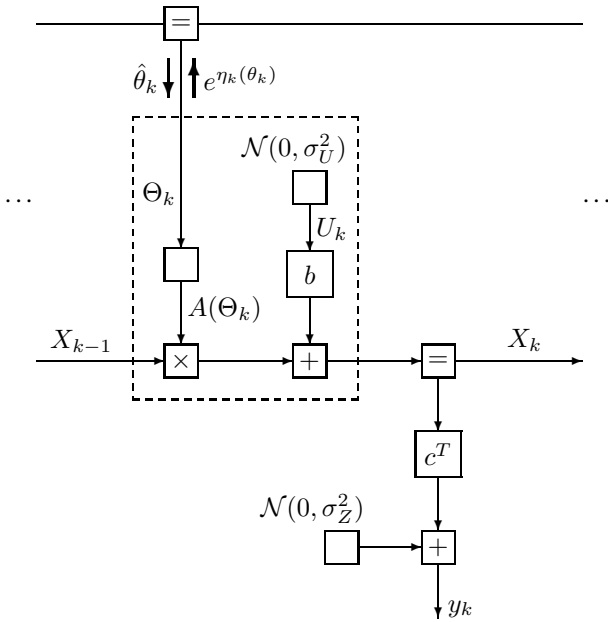


Fig. 5. Linear state space model for autoregressive filter with $b = c = (1, 0, \dots, 0)^T$, with unknown coefficient vector Θ , and with scalar white Gaussian innovation U_1, U_2, \dots . The figure shows one section of the factor graph. The multiplier node denotes the product $A(\Theta)X_k$ (50). The EM message computation rule (III.7) and (III.8) applies to the dashed box.

- 2) The point of these examples is only to illustrate the message passing view of the EM algorithm; we are not concerned here with analyzing and comparing different approaches to linear-system identification [31].
- 3) Tabulated message computation rules (as in Table II) can greatly simplify the derivation of EM message passing algorithms.

V. GAUSSIAN MESSAGE PASSING THROUGH MULTIPLIER NODES

A substantial part of traditional signal processing is essentially equivalent to Gaussian message passing in linear models [5]. Unknown coefficients in such models introduce multiplier nodes into the corresponding factor graphs as is exemplified by Figures 4 and 5.

The EM message out of such multiplier nodes, properly grouped with “soft” Gaussian nodes/factors as in Figures 4 and 5, is invariably Gaussian (up to a scale factor), but the computation of its mean and its covariance matrix (in terms of the parameters of the incoming Gaussian messages) can be involved, cf. Appendices C–E. It is therefore helpful to tabulate such messages as exemplified by Table II.

However, such multiplier nodes come in surprisingly many versions: scalar times scalar, scalar times vector, inner product of two vectors (as in Fig. 4), general matrix times vector, products involving matrices with a special structure (as in Fig. 5), etc. Moreover, the grouping of such multiplier nodes with suitable soft factors/nodes is another source of virtually endless variety.

We will therefore confine ourselves to a small number of cases which appear to be particularly useful and widely

applicable. The general setup is shown in Table III and the results are given in Tables III and IV. In all cases, we have a multiplier $U = A(\Theta)X$, where $A(\Theta)$ is a matrix that depends on Θ , grouped with $Y = U + Z$, where Z is zero-mean Gaussian with covariance matrix $V_Z = W_Z^{-1}$ (or σ_Z^2 in the scalar case). In all cases, we assume that Gaussian messages $\vec{\mu}_X$ and $\vec{\mu}_Y$ arrive via the edges X and Y , respectively; these incoming messages are parameterized by the mean vectors \vec{m}_X and \vec{m}_Y and the covariance matrices $\vec{V}_X = \vec{W}_X^{-1}$ and $\vec{V}_Y = \vec{W}_Y^{-1}$, respectively. The following cases are considered:

- 1) Inner product: $A(\Theta) = \Theta^T$, both Θ and X are real column vectors (of the same dimension), and both $U = \Theta^T X$ and Y are real scalars. This case is a generalization of Table II, as will be discussed at the end of this section.
- 2) Real scalar Θ times real column vector X : $A(\Theta) = \Theta$ and both $U = \Theta X$ and Y are column vectors. Some pertinent properties of the trace operator (“tr”) are recalled in Appendix B.
- 3) Componentwise product (denoted by $\Theta \odot X$) of real column vectors Θ and X : $A(\Theta) = \text{diag}(\Theta)$, a diagonal matrix with the elements of Θ on the diagonal, and both $U = \Theta \odot X$ and Y are column vectors.
- 4) Autoregression: Θ, X, Y are column vectors in \mathbb{R}^n and $A(\Theta)$ is the square matrix (50) (which is essentially a companion matrix). In addition, Z is a zero-mean Gaussian vector with covariance matrix

$$V_Z = \begin{pmatrix} \sigma_Z^2 & 0 & \dots & 0 \\ 0 & 0 & & \vdots \\ \vdots & & \ddots & \\ \vdots & & & \ddots \end{pmatrix}, \quad (54)$$

i.e., Z is effectively a scalar that affects only the first component Y_1 of Y .

- 5) General real matrix Θ times real column vector X : $A(\Theta) = \Theta$ and both $U = \Theta X$ and Y are column vectors.

The symbol “ \otimes ” in (III.9) and (III.10) denotes the Kronecker product, cf. (124)–(125). More about this case is said below.

The case of scalar Θ times scalar X is a common special case of all these cases and does not need to be considered separately.

In the cases 1–4, where Θ is a column vector (or a scalar), the EM message $e^{\eta(\theta)}$ is Gaussian with mean vector \vec{m}_Θ and weight matrix (inverse covariance matrix) \vec{W}_Θ as given in Table III.

In Case 5, where Θ is a matrix, we need the following notation. Let B be any $m \times n$ matrix and let

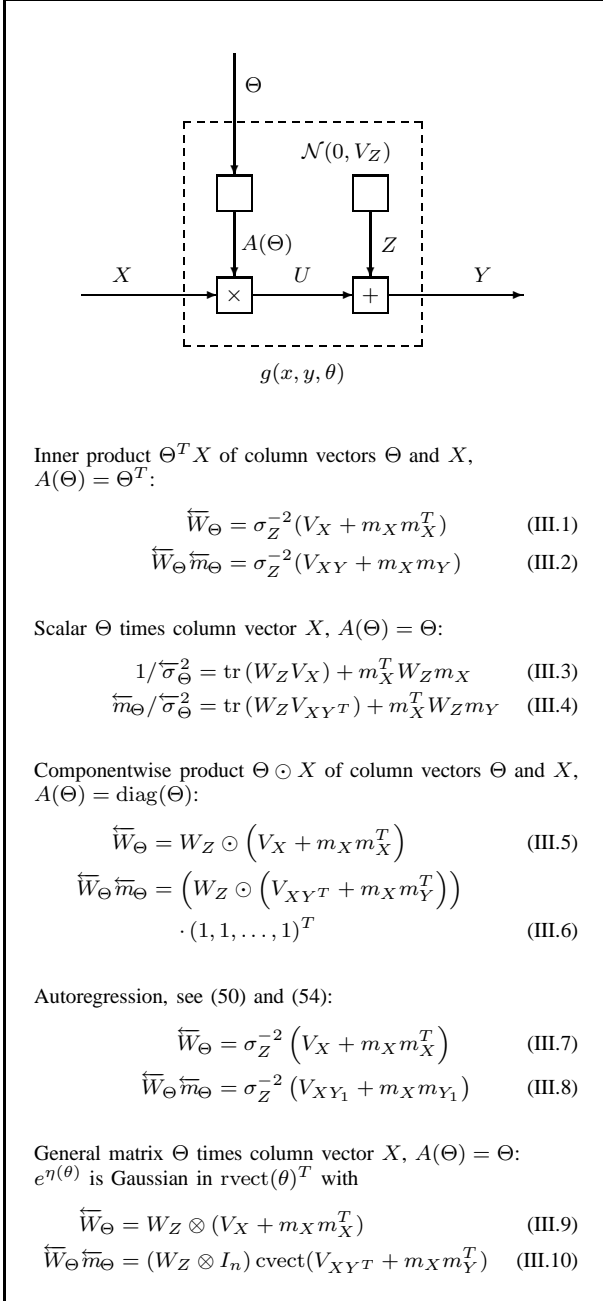
$$B = \begin{pmatrix} b_1 \\ \vdots \\ b_m \end{pmatrix} \quad (55)$$

be the decomposition of B into its rows. We will use both the row stack vector

$$\text{rvect}(B) \triangleq (b_1, \dots, b_m) \quad (56)$$

TABLE III

GAUSSIAN BACKWARD EM MESSAGES $e^{\eta(\theta)}$ THROUGH SOME MULTIPLIER NODES, SEE SECTION V. THE EM MESSAGE $e^{\eta(\theta)}$ IS ALWAYS GAUSSIAN (UP TO A CONSTANT SCALE FACTOR) WITH PARAMETERS \overleftarrow{W}_Θ AND \overleftarrow{m}_Θ AS STATED. SEE ALSO TABLE IV.



and the analogous column stack vector $\text{cvect}(B)$, where the columns of B are stacked into one column vector. For example, if

$$B = \begin{pmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{pmatrix} \quad (57)$$

then $\text{rvect}(B) = (b_{1,1}, b_{1,2}, b_{2,1}, b_{2,2})$ and $\text{cvect}(B) = (b_{1,1}, b_{2,1}, b_{1,2}, b_{2,2})^T$. With this notation, the EM message is Gaussian in $\text{rvect}(\Theta)^T$ with parameters (III.9) and (III.10) (see also (132)).

Note that Table III gives the analog of (II.1) and (II.2) in

TABLE IV

COMPUTATION OF MEANS m_X AND m_Y AND COVARIANCE MATRICES V_X AND V_{XY^T} IN TABLE III.

Auxiliary quantities:

$$W_X = \overleftarrow{W}_X + A(\hat{\theta})^T (V_Z + \overleftarrow{V}_Y)^{-1} A(\hat{\theta}) \quad (\text{IV.1})$$

$$\overleftarrow{V}_Y = A(\hat{\theta}) \overleftarrow{V}_X A(\hat{\theta})^T + V_Z \quad (\text{IV.2})$$

$$\overleftarrow{W}_Y = (\overleftarrow{V}_Y + \overleftarrow{V}_Y)^{-1} \quad (\text{IV.3})$$

Quantities in Table III:

$$V_X = W_X^{-1} \quad (\text{IV.4})$$

$$= \overleftarrow{V}_X - \overleftarrow{V}_X A(\hat{\theta})^T \overleftarrow{W}_Y A(\hat{\theta}) \overleftarrow{V}_X \quad (\text{IV.5})$$

$$V_{XY^T} = \overleftarrow{V}_X A(\hat{\theta})^T \overleftarrow{W}_Y \overleftarrow{V}_Y \quad (\text{IV.6})$$

$$m_X = V_X \left(\overleftarrow{W}_X \overleftarrow{m}_X + A(\hat{\theta})^T (V_Z + \overleftarrow{V}_Y)^{-1} \overleftarrow{m}_Y \right) \quad (\text{IV.7})$$

$$= (I_n - \overleftarrow{V}_X A(\hat{\theta})^T \overleftarrow{W}_Y A(\hat{\theta})) \cdot \left(\overleftarrow{m}_X + \overleftarrow{V}_X A(\hat{\theta})^T (V_Z + \overleftarrow{V}_Y)^{-1} \overleftarrow{m}_Y \right) \quad (\text{IV.8})$$

$$m_Y = V_Y (\overleftarrow{W}_Y \overleftarrow{m}_Y + \overleftarrow{W}_Y \overleftarrow{m}_Y) \quad (\text{IV.9})$$

$$= (I_m - \overleftarrow{V}_Y \overleftarrow{W}_Y) (\overleftarrow{m}_Y + \overleftarrow{V}_Y \overleftarrow{W}_Y \overleftarrow{m}_Y) \quad (\text{IV.10})$$

Table II; the analog of (II.3) and (II.4) is Table IV, which gives expressions for the marginal means m_X and m_Y and for the covariance matrices V_X and V_{XY^T} for fixed $\Theta = \hat{\theta}$ in terms of the parameters \overleftarrow{m}_X and \overleftarrow{V}_X and \overleftarrow{m}_Y and \overleftarrow{V}_Y of the incoming Gaussian sum-product messages. Note that Table IV applies to all the cases in Table III simultaneously.

The proofs of the claims in Table III are given in Appendix C and the proofs of the claims in Table IV are given in appendices D and E. Not surprisingly, some of these derivations are essentially equivalent to similar computations in the EM literature [33]–[35]. Nevertheless, most of the statements in Tables III and IV do not seem to be readily available in the prior literature.

We conclude this section by considering the specialization of Case 1 (inner product) to $Y = y$ fixed, which results in the situation of Table II. In this case, we have

$$m_Y = \overleftarrow{m}_y = y \quad (58)$$

and

$$V_{XY} = V_Y = \overleftarrow{V}_Y = 0. \quad (59)$$

With the translations $m_S = m_Y$ and $\sigma_S^2 = \sigma_Z^2$, it is obvious that (III.1) and (III.2) specialize to (II.1) and (II.2), respectively. Moreover, with $A(\hat{\theta})^T = \hat{\theta}$, it is obvious that (II.3) follows from (IV.1) and (II.4) follows from (IV.7).

VI. CONCLUSIONS

We have showed that EM may be viewed and used as a message passing algorithm in factor graphs, and we have

identified a general “local” EM message computation rule (Table I). In some important cases, the EM messages are tractable expressions, which was exemplified by the EM message out of multipliers (arising from unknown coefficients) in linear Gaussian models. □

As a full member of the family of message passing algorithms, it is easy to seamlessly combine expectation maximization with other message passing algorithms in interesting ways. In particular:

- EM messages (like all messages) may be represented in many different ways (including Gaussians as in Sections IV and V, Gaussian mixtures [28], particles [32], etc., leading to quite different actual computations.
- The freedom (or the necessity) to choose some definite message update schedule leads to different algorithms with different performance; more about this will be said in [28].
- The maximization step amounts to applying the max-product algorithm to the corresponding subgraph, which in turn may be carried out by many (exact or approximate) message passing algorithms. For example, in some important applications (as, e.g., in Section IV), the maximization step can be done by Kalman filtering/smoothing.
- The expectation step relies on plain sum-product messages. However, depending on the involved nodes and message types, the sum-product algorithm may be realized (exactly or approximately) in many different ways, cf. [5, Section VI].

Moreover, it is a general observation that tabulated message computation rules can greatly simplify the derivation of message passing algorithms [5]. This applies, in particular, to EM messages, which we have tabulated for various multiplier nodes (scalar, vector, general matrix, ...) with incoming Gaussian messages. With these message tables, EM algorithms for a number of basic linear-system identification problems can easily be composed without additional derivations or computations. More such tables will be given in [28].

APPENDIX A PROOF OF EQUATION (6)

We give a variation of a standard proof (cf. [9]) that is adapted to the setup of Section II. The heart of the proof is the following fact.

Lemma: The function

$$\tilde{f}(\theta, \hat{\theta}) \triangleq f(\hat{\theta}) + \int_x f(x, \hat{\theta}) \log \left(\frac{f(x, \theta)}{f(x, \hat{\theta})} \right) dx \quad (60)$$

(where “log” denotes the natural logarithm) satisfies both

$$\tilde{f}(\theta, \hat{\theta}) \leq f(\theta) \quad (61)$$

and

$$\tilde{f}(\theta, \theta) = f(\theta). \quad (62)$$

Proof: The equality (62) is obvious. The inequality (61) follows from eliminating the logarithm in (60) by the inequality $\log(x) \leq x - 1$ for $x > 0$:

$$\tilde{f}(\theta, \hat{\theta}) \leq f(\hat{\theta}) + \int_x f(x, \hat{\theta}) \left(\frac{f(x, \theta)}{f(x, \hat{\theta})} - 1 \right) dx \quad (63)$$

$$= f(\hat{\theta}) + \int_x f(x, \theta) dx - \int_x f(x, \hat{\theta}) dx \quad (64)$$

$$= f(\theta). \quad (65)$$

■

To prove (6), we first note that (5) is equivalent to

$$\hat{\theta}^{(k+1)} = \operatorname{argmax}_{\theta} \tilde{f}(\theta, \hat{\theta}^{(k)}). \quad (66)$$

We then obtain

$$f(\hat{\theta}^{(k)}) = \tilde{f}(\hat{\theta}^{(k)}, \hat{\theta}^{(k)}) \quad (67)$$

$$\leq \tilde{f}(\hat{\theta}^{(k+1)}, \hat{\theta}^{(k)}) \quad (68)$$

$$\leq f(\hat{\theta}^{(k+1)}), \quad (69)$$

where (67) follows from (62), (68) follows from (66), and (69) follows from (61).

APPENDIX B SOME PROPERTIES OF THE TRACE OPERATOR

We recall some pertinent properties of the trace operator for use in Appendix C-B. The entries of a matrix A will be denoted by $a_{k,\ell}$. The trace of a square matrix A is the sum of the diagonal elements of A :

$$\operatorname{tr}(A) \triangleq \sum_k a_{k,k}. \quad (70)$$

For matrices A and B such that AB is a square matrix (i.e., B has the same dimensions as A^T), we have

$$\operatorname{tr}(AB) = \sum_k \sum_{\ell} a_{k,\ell} b_{\ell,k} \quad (71)$$

$$= \operatorname{tr}(BA). \quad (72)$$

In particular, if x and y are column vectors (with the same number of rows), we have

$$x^T y = y^T x = \operatorname{tr}(xy^T). \quad (73)$$

Moreover, for $W = A^T A$, we have

$$x^T W y = (Ax)^T Ay \quad (74)$$

$$= \operatorname{tr}(Ax(Ay)^T) \quad (75)$$

$$= \operatorname{tr}(Axy^T A^T), \quad (76)$$

and using (72) we further obtain

$$x^T W y = \operatorname{tr}(Wxy^T) \quad (77)$$

$$= \operatorname{tr}(xy^T W). \quad (78)$$

Now let X and Y be random column vectors with the same dimensions. Let $m_X \triangleq \mathbb{E}[X]$ and $m_Y \triangleq \mathbb{E}[Y]$ and

$$V_{XY^T} \triangleq \mathbb{E}[(X - m_X)(Y - m_Y)^T]. \quad (79)$$

Then, for any square matrix W as above (i.e., $W = A^T A$) with suitable dimensions, we have

$$\begin{aligned} \mathbb{E}[X^T W Y] &= \mathbb{E}[(X - m_X)^T W (Y - m_Y)] + m_X^T W m_Y \quad (80) \\ &= \mathbb{E}[\text{tr}(W(X - m_X)(Y - m_Y)^T)] + m_X^T W m_Y \quad (81) \\ &= \text{tr}(W V_{XY^T}) + m_X^T W m_Y. \quad (82) \end{aligned}$$

APPENDIX C PROOFS OF THE CLAIMS IN TABLE III

Recall (for repeated use below) that the probability density function of an n -dimensional real Gaussian random vector

$$f(x) = \frac{1}{(2\pi)^n} \sqrt{\det(W)} e^{-\frac{1}{2}(x-m)^T W (x-m)} \quad (83)$$

$$\propto e^{-\frac{1}{2}(x^T W x - 2x^T W m)}, \quad (84)$$

where m is the mean vector and $W = V^{-1}$ (a positive definite matrix) is the inverse of the covariance matrix V . In the scalar case ($n = 1$), we will also use the notation $\sigma^2 \triangleq V$.

Now consider the factor graph in Table III. The closed-box function $g(x, y, \theta)$ is obtained by marginalization/integration over the variables inside the dashed box:

$$\begin{aligned} g(x, y, \theta) &= \int_u \delta(u - A(\theta)x) \sqrt{\frac{\det(W_Z)}{(2\pi)^n}} e^{-\frac{1}{2}(y-u)^T W_Z (y-u)} du \quad (85) \\ &= \sqrt{\frac{\det(W_Z)}{(2\pi)^n}} e^{-\frac{1}{2}(y-A(\theta)x)^T W_Z (y-A(\theta)x)}. \quad (86) \end{aligned}$$

The exponent (I.1) of the EM message $e^{\eta(\theta)}$ is

$$\eta(\theta) = \mathbb{E}[\log g(X, Y, \theta)] \quad (87)$$

$$\begin{aligned} &= \frac{1}{2} \log \left(\frac{\det(W_Z)}{(2\pi)^n} \right) \\ &\quad - \frac{1}{2} \mathbb{E}[(Y - A(\theta)X)^T W_Z (Y - A(\theta)X)] \quad (88) \\ &= \text{const} - \frac{1}{2} \left(\mathbb{E}[(A(\theta)X)^T W_Z (A(\theta)X)] \right. \\ &\quad \left. - 2\mathbb{E}[(A(\theta)X)^T W_Z Y] \right), \quad (89) \end{aligned}$$

where all logarithms are natural, where the expectation is over X and Y (with respect to the local probability (137)), and where ‘‘const’’ subsumes all terms that do not depend on θ .

We are now ready to discuss the individual cases of Table III.

A. Inner Product $\Theta^T X$ of Column Vectors Θ and X

In this case, we have $A(\theta) = \theta^T$. The quantities $\theta^T X$, Y , and W_Z are scalars; in particular, $(\theta^T X)^T = \theta^T X$. Thus (89)

becomes

$$\begin{aligned} \eta(\theta) &= -\frac{1}{2} \left(\mathbb{E}[(\theta^T X)^T W_Z (\theta^T X)] - 2\mathbb{E}[(\theta^T X)^T W_Z Y] \right) \\ &\quad + \text{const} \quad (90) \end{aligned}$$

$$\begin{aligned} &= -\frac{1}{2} \left(\mathbb{E}[\theta^T X W_Z X^T \theta] - 2\mathbb{E}[\theta^T X W_Z Y] \right) \\ &\quad + \text{const} \quad (91) \end{aligned}$$

$$\begin{aligned} &= -\frac{1}{2} \left(\theta^T \mathbb{E}[X W_Z X^T] \theta - 2\theta^T \mathbb{E}[X W_Z Y] \right) \\ &\quad + \text{const.} \quad (92) \end{aligned}$$

It is then obvious from (84) that the EM message $e^{\eta(\theta)}$ is Gaussian (up to a scale factor) with weight matrix

$$\overleftarrow{W}_\Theta = \mathbb{E}[X X^T] \sigma_Z^{-2} \quad (93)$$

$$= \frac{V_X + m_X m_X^T}{\sigma_Z^2} \quad (94)$$

and

$$\overleftarrow{W}_\Theta \overleftarrow{m}_\Theta = \mathbb{E}[X Y] \sigma_Z^{-2} \quad (95)$$

$$= \frac{V_{XY} + m_X m_Y}{\sigma_Z^2} \quad (96)$$

B. Scalar Θ Times Column Vector X

In this case, we have $A(\theta) = \theta$, a scalar, and (89) becomes

$$\eta(\theta) = \text{const} - \frac{1}{2} \left(\theta^2 \mathbb{E}[X^T W_Z X] - 2\theta \mathbb{E}[X^T W_Z Y] \right). \quad (97)$$

It follows from (84) that $e^{\eta(\theta)}$ is Gaussian with

$$\overleftarrow{\sigma}_\Theta^{-2} = \mathbb{E}[X^T W_Z X] \quad (98)$$

$$= \text{tr}(W_Z V_X) + m_X^T W_Z m_X \quad (99)$$

and

$$\overleftarrow{m}_\Theta / \overleftarrow{\sigma}_\Theta = \mathbb{E}[X^T W_Z Y] \quad (100)$$

$$= \text{tr}(W_Z V_{XY^T}) + m_X^T W_Z m_Y \quad (101)$$

where (99) and (101) follow from (82) and with V_{XY^T} defined as in (155).

C. Componentwise Product $\Theta \odot X$ of Column Vectors

In this case, we have $A(\theta) = \text{diag}(\theta)$, a diagonal matrix with the elements of θ on the diagonal, and (89) becomes

$$\begin{aligned} \eta(\theta) &= \text{const} - \frac{1}{2} \left(\mathbb{E}[(\text{diag}(\theta)X)^T W_Z (\text{diag}(\theta)X)] \right. \\ &\quad \left. - 2\mathbb{E}[(\text{diag}(\theta)X)^T W_Z Y] \right) \quad (102) \end{aligned}$$

$$\begin{aligned} &= \text{const} - \frac{1}{2} \left(\mathbb{E}[(\text{diag}(X)\theta)^T W_Z (\text{diag}(X)\theta)] \right. \\ &\quad \left. - 2\mathbb{E}[(\text{diag}(X)\theta)^T W_Z Y] \right) \quad (103) \end{aligned}$$

$$\begin{aligned} &= \text{const} - \frac{1}{2} \left(\theta^T \mathbb{E}[\text{diag}(X) W_Z \text{diag}(X)] \theta \right. \\ &\quad \left. - 2\theta^T \mathbb{E}[\text{diag}(X) W_Z Y] \right). \quad (104) \end{aligned}$$

It follows from (84) that $e^{\eta(\theta)}$ is Gaussian with

$$\overleftarrow{W}_\Theta = \mathbb{E}[\text{diag}(X) W_Z \text{diag}(X)] \quad (105)$$

$$= W_Z \odot \mathbb{E}[X X^T] \quad (106)$$

$$= W_Z \odot (V_X + m_X m_X^T) \quad (107)$$

and

$$\overleftarrow{W}_\Theta \overleftarrow{m}_\Theta = \mathbb{E}[\text{diag}(X)W_Z Y] \quad (108)$$

$$= \mathbb{E}\left[\text{diag}(X)W_Z \text{diag}(Y) (1, 1, \dots, 1)^T\right] \quad (109)$$

$$= (W_Z \odot \mathbb{E}[XY^T]) (1, 1, \dots, 1)^T \quad (110)$$

$$= (W_Z \odot (V_{XY^T} + m_X m_Y^T)) (1, 1, \dots, 1)^T. \quad (111)$$

D. Autoregression (Companion Matrix)

In this case, recall from (50) that

$$A(\theta) \triangleq \begin{pmatrix} \theta^T & \\ I_{n-1} & 0 \end{pmatrix} \quad (112)$$

where n is the dimension of the column vector θ , and where I_{n-1} is the $(n-1) \times (n-1)$ identity matrix.

Before we proceed, we need to address the following issue. According to (54), we have

$$V_Z = \begin{pmatrix} \sigma_Z^2 & 0 & 0 & \dots & 0 \\ 0 & \varepsilon & 0 & \dots & 0 \\ 0 & 0 & \varepsilon & \dots & \\ \dots & & & & \end{pmatrix} \quad (113)$$

with $\varepsilon = 0$, which creates a problem with $W_Z = V_Z^{-1}$. We address this problem by proceeding with (113) with $\varepsilon > 0$. As it turns out, the resulting expression for $\eta(\theta)$ does not depend on ε (except in an additive constant, which we ignore).

Using (112), (89) becomes

$$\eta(\theta) = \text{const} - \frac{1}{2} \left(\mathbb{E} \left[\begin{pmatrix} \theta^T X \\ X_1 \\ \vdots \\ X_{n-1} \end{pmatrix}^T W_Z \begin{pmatrix} \theta^T X \\ X_1 \\ \vdots \\ X_{n-1} \end{pmatrix} \right] - 2 \mathbb{E} \left[\begin{pmatrix} \theta^T X \\ X_1 \\ \vdots \\ X_{n-1} \end{pmatrix}^T W_Z Y \right] \right). \quad (114)$$

Using (113) and ignoring all constant terms yields

$$\eta(\theta) = \text{const} - \frac{1}{2} \left(\mathbb{E}[\theta^T X \sigma_Z^{-2} \theta^T X] - 2 \mathbb{E}[\theta^T X \sigma_Z^{-2} Y_1] \right) \quad (115)$$

$$= \text{const} - \frac{1}{2} \left(\theta^T \sigma_Z^{-2} \mathbb{E}[X X^T] \theta - 2 \theta^T \sigma_Z^{-2} \mathbb{E}[X Y_1] \right). \quad (116)$$

It follows from (84) that $e^{\eta(\theta)}$ is Gaussian with

$$\overleftarrow{W}_\Theta = \sigma_Z^{-2} \mathbb{E}[X X^T] \quad (117)$$

$$= \sigma_Z^{-2} (V_X + m_X m_X^T) \quad (118)$$

and

$$\overleftarrow{W}_\Theta \overleftarrow{m}_\Theta = \sigma_Z^{-2} \mathbb{E}[X Y_1] \quad (119)$$

$$= \sigma_Z^{-2} (V_{X Y_1} + m_X m_{Y_1}^T). \quad (120)$$

E. General Matrix Θ Times Column Vector X

We need to begin with some preparations. Recall the row stack operator rvect (56) and the corresponding column stack operators cvect . Let A be an $m \times n$ matrix with rows a_1, \dots, a_m . For any column vector $x \in \mathbb{R}^n$ and any $m \times m$ square matrix W (with elements $w_{k,\ell}$), we have

$$(Ax)^T W Ax = (a_1 x, \dots, a_m x) W \begin{pmatrix} a_1 x \\ \vdots \\ a_m x \end{pmatrix} \quad (121)$$

$$= \sum_{k=1}^m \sum_{\ell=1}^m a_k x w_{k,\ell} (a_\ell x) \quad (122)$$

$$= \sum_{k=1}^m \sum_{\ell=1}^m a_k w_{k,\ell} x x^T a_\ell^T \quad (123)$$

$$= (a_1, \dots, a_m) \cdot \begin{pmatrix} w_{1,1} x x^T & \dots & w_{1,m} x x^T \\ \vdots & & \vdots \\ w_{m,1} x x^T & \dots & w_{m,m} x x^T \end{pmatrix} \begin{pmatrix} a_1^T \\ \vdots \\ a_m^T \end{pmatrix} \quad (124)$$

$$= \text{rvect}(A) (W \otimes x x^T) \text{rvect}(A)^T. \quad (125)$$

Moreover, for any column vector $y \in \mathbb{R}^m$, we have

$$(Ax)^T W y = (a_1 x, \dots, a_m x) W \begin{pmatrix} y_1 \\ \vdots \\ y_m \end{pmatrix} \quad (126)$$

$$= \sum_{k=1}^m \sum_{\ell=1}^m a_k x w_{k,\ell} y_\ell \quad (127)$$

$$= \sum_{k=1}^m \sum_{\ell=1}^m a_k w_{k,\ell} x y_\ell \quad (128)$$

$$= (a_1, \dots, a_m) \cdot \begin{pmatrix} w_{1,1} I_n & \dots & w_{1,m} I_n \\ \vdots & & \vdots \\ w_{m,1} I_n & \dots & w_{m,m} I_n \end{pmatrix} \begin{pmatrix} x y_1 \\ \vdots \\ x y_m \end{pmatrix} \quad (129)$$

$$= \text{rvect}(A) (W \otimes I_n) \text{cvect}(x y^T). \quad (130)$$

After these preparations, we return to the EM message for the case where $A(\theta) = \Theta$ is a general $m \times n$ matrix. In this case, (89) becomes

$$\eta(\Theta) = \text{const} - \frac{1}{2} \left(\mathbb{E}[(\Theta X)^T W_Z (\Theta X)] - 2 \mathbb{E}[(\Theta X)^T W_Z Y] \right) \quad (131)$$

and using (125) and (130) we obtain

$$\eta(\Theta) = \text{const} - \frac{1}{2} \left(\text{rvect}(\Theta) \mathbb{E}[W_Z \otimes X X^T] \text{rvect}(\Theta)^T - 2 \text{rvect}(\Theta) \mathbb{E}[(W_Z \otimes I_n) \text{cvect}(X Y^T)] \right). \quad (132)$$

We now see that $e^{\eta(\Theta)}$ is Gaussian in $\text{rvect}(\Theta)^T$ with

$$\overleftarrow{W}_\Theta = W_Z \otimes \mathbb{E}[X X^T] \quad (133)$$

$$= W_Z \otimes (V_X + m_X m_X^T) \quad (134)$$

and

$$\overleftarrow{W}_\Theta \overleftarrow{m}_\Theta = (W_Z \otimes I_n) \text{cvect}(\mathbb{E}[X Y^T]) \quad (135)$$

$$= (W_Z \otimes I_n) \text{cvect}(V_{X Y^T} + m_X m_Y^T). \quad (136)$$

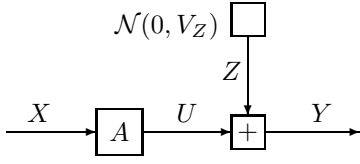


Fig. 6. Factor graph for Appendix D.

APPENDIX D

PROOFS OF THE CLAIMS IN TABLE IV EXCEPT (IV.6)

We consider the computation of the mean vectors m_X and m_Y and the covariance matrix V_X with respect to the local probability density (I.3)

$$p_{\text{local}}(x, y | \hat{\theta}) \propto g(x, y, \hat{\theta}) \vec{\mu}_X(x) \overleftarrow{\mu}_Y(y) \quad (137)$$

with $g(x, y, \theta)$ as in Table III (see also (86)) and where $\vec{\mu}_X$ and $\overleftarrow{\mu}_Y$ are the incoming Gaussian sum-product messages with parameters \vec{m}_X and \vec{V}_X (or $\vec{W}_X = \vec{V}_X^{-1}$) and \overleftarrow{m}_Y and \overleftarrow{V}_Y (or $\overleftarrow{W}_Y = \overleftarrow{V}_Y^{-1}$), respectively.

Throughout this section, $\Theta = \hat{\theta}$ is fixed and we will simply write A instead of $A(\hat{\theta})$. The factor graph of Table III then reduces to the factor graph of Fig. 6. The desired quantities may be obtained by Gaussian sum-product message passing in this factor graph. In the following computations, we will frequently use Tables 2 and 3 of [5] without special notice; the reader is advised to have these tables at hand.

Equation (IV.1) follows from

$$W_X = \vec{W}_X + \overleftarrow{W}_X \quad (138)$$

$$= \vec{W}_X + A^T \overleftarrow{W}_U A \quad (139)$$

$$= \vec{W}_X + A^T (V_Z + \overleftarrow{V}_Y)^{-1} A. \quad (140)$$

Equation (IV.2) is immediate from

$$\vec{V}_Y = \vec{V}_U + V_Z \quad (141)$$

$$= A \vec{V}_X A^T + V_Z. \quad (142)$$

Equation (IV.3) is the definition of \vec{W} as in [5, eq. (56)].

Equation (IV.5) follows from [5, (I.4) and (III.8)]:

$$V_X = \vec{V}_X - \vec{V}_X \vec{W}_X \vec{V}_X \quad (143)$$

$$= \vec{V}_X - \vec{V}_X A^T \overleftarrow{W}_Y A \vec{V}_X. \quad (144)$$

Equation (IV.7) follows from

$$W_X m_X = \vec{W}_X \vec{m}_X + \overleftarrow{W}_X \overleftarrow{m}_X \quad (145)$$

$$= \vec{W}_X \vec{m}_X + A^T \overleftarrow{W}_U \overleftarrow{m}_U \quad (146)$$

$$= \vec{W}_X \vec{m}_X + A^T (V_Z + \overleftarrow{V}_Y)^{-1} \overleftarrow{m}_Y. \quad (147)$$

Using (144) and (147), Equation (IV.8) follows from

$$m_X = V_X W_X m_X \quad (148)$$

$$= \left(\vec{V}_X - \vec{V}_X A^T \overleftarrow{W}_Y A \vec{V}_X \right) \cdot \left(\vec{W}_X \vec{m}_X + A^T (V_Z + \overleftarrow{V}_Y)^{-1} \overleftarrow{m}_Y \right) \quad (149)$$

$$= \left(I_n - \vec{V}_X A^T \overleftarrow{W}_Y A \right) \cdot \left(\vec{m}_X + \vec{V}_X A^T (V_Z + \overleftarrow{V}_Y)^{-1} \overleftarrow{m}_Y \right). \quad (150)$$

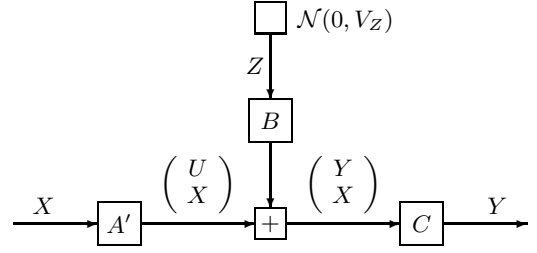


Fig. 7. Factor graph for Appendix E.

Equation (IV.9) is immediate from

$$W_Y m_Y = \vec{W}_Y \vec{m}_Y + \overleftarrow{W}_Y \overleftarrow{m}_Y. \quad (151)$$

Finally, Equation (IV.10), is obtained using [5, (eq. I.4)]:

$$m_Y = V_Y W_Y m_Y \quad (152)$$

$$= \left(\vec{V}_Y - \vec{V}_Y \overleftarrow{W}_Y \vec{V}_Y \right) \left(\vec{W}_Y \vec{m}_Y + \overleftarrow{W}_Y \overleftarrow{m}_Y \right) \quad (153)$$

$$= \left(I_m - \vec{V}_Y \overleftarrow{W}_Y \right) \left(\overleftarrow{m}_Y + \vec{V}_Y \overleftarrow{W}_Y \overleftarrow{m}_Y \right). \quad (154)$$

APPENDIX E

PROOF OF (IV.6)

We need to compute the covariance matrix

$$V_{XY^T} \triangleq E[(X - m_X)(Y - m_Y)^T] \quad (155)$$

with respect to the local probability density (137). Consider the factor graph shown in Fig. 7 with block matrices

$$A' \triangleq \begin{pmatrix} A \\ I_n \end{pmatrix}, \quad (156)$$

$$B \triangleq \begin{pmatrix} I_m \\ 0 \end{pmatrix}, \quad (157)$$

$$C \triangleq (I_m, 0), \quad (158)$$

where n and m are the dimensions of the column vectors X and Y , respectively. This factor graph is obtained from the factor graph in Table III by stretching the variable X across the adder node so that the variables X and Y now appear jointly as components of the vector $(Y^T, X^T)^T$ on the correspondingly labeled edge. The closed-box function $g(x, y)$ in Fig. 7 equals the closed-box function $g(x, y, \hat{\theta})$ in the factor graph in Table III.

The desired matrix V_{XY^T} is the lower left corner of the covariance matrix

$$V_{\begin{pmatrix} Y \\ X \end{pmatrix}} = \begin{pmatrix} V_Y & V_{XY^T} \\ V_{XY^T} & V_X \end{pmatrix}, \quad (159)$$

which can be computed by Gaussian sum-product message passing in Fig. 7. As in Appendix D, we will use Tables 2 and 3 of [5] without special notice. We have

$$\vec{V}_{\begin{pmatrix} U \\ X \end{pmatrix}} = A' \vec{V}_X (A')^T \quad (160)$$

$$= \begin{pmatrix} A \vec{V}_X A^T & A \vec{V}_X \\ \vec{V}_X A^T & \vec{V}_X \end{pmatrix} \quad (161)$$

and

$$\vec{V}_{(x)} = \vec{V}_{(x)} + BV_Z B^T \quad (162)$$

$$= \begin{pmatrix} A\vec{V}_X A^T + V_Z & A\vec{V}_X \\ \vec{V}_X A^T & \vec{V}_X \end{pmatrix}. \quad (163)$$

We also have

$$W_{(x)} = \vec{W}_{(x)} + \overleftarrow{W}_{(x)} \quad (164)$$

$$= \vec{V}_{(x)}^{-1} + C^T \overleftarrow{V}_Y^{-1} C \quad (165)$$

and the Matrix Inversion Lemma (see, e.g., [5, eq. (181)]) yields

$$V_{(x)} = \vec{V}_{(x)} - \vec{V}_{(x)} C^T \cdot \left(\overleftarrow{V}_Y + C \vec{V}_{(x)} C^T \right)^{-1} C \vec{V}_{(x)} \quad (166)$$

$$= \vec{V}_{(x)} - \vec{V}_{(x)} C^T \cdot \left(\overleftarrow{V}_Y + A \vec{V}_X A^T + V_Z \right)^{-1} C \vec{V}_{(x)} \quad (167)$$

$$= \vec{V}_{(x)} - \begin{pmatrix} A \vec{V}_X A^T + V_Z \\ \vec{V}_X A^T \end{pmatrix} \cdot \left(\overleftarrow{V}_Y + A \vec{V}_X A^T + V_Z \right)^{-1} \cdot \left(A \vec{V}_X A^T + V_Z, A \vec{V}_X \right). \quad (168)$$

The lower left corner of this matrix is

$$V_{XY^T} = \vec{V}_X A^T - \vec{V}_X A^T \left(\overleftarrow{V}_Y + A \vec{V}_X A^T + V_Z \right)^{-1} \cdot \left(A \vec{V}_X A^T + V_Z \right) \quad (169)$$

$$= \vec{V}_X A^T \left(\overleftarrow{V}_Y + A \vec{V}_X A^T + V_Z \right)^{-1} \cdot \left(\left(\overleftarrow{V}_Y + A \vec{V}_X A^T + V_Z \right) - \left(A \vec{V}_X A^T + V_Z \right) \right) \quad (170)$$

$$= \vec{V}_X A^T \left(A \vec{V}_X A^T + V_Z + \overleftarrow{V}_Y \right)^{-1} \overleftarrow{V}_Y \quad (171)$$

and using

$$\tilde{W}_Y = \left(A \vec{V}_X A^T + V_Z + \overleftarrow{V}_Y \right)^{-1} \quad (172)$$

from (IV.3) and (IV.2) yields (IV.6).

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