

Univariate Exponentially Modified Gaussian Wave Mixture Model Optimization

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This document elaborates on a closed-form analytical solution to an Exponentially-Modified Gaussian (EMG) mixture model using least-squares optimization.

1 Objective

Let the Exponentially Modified Gaussian (EMG) be

$$m(\mathbf{p}; \mathbf{x}) = m(\alpha, \mu, \sigma, \lambda; \mathbf{x}) = \alpha \mathcal{N}(\mathbf{x}|\mu, \sigma) \Phi(\mathbf{x}|\lambda, \mu, \sigma) A(\mathbf{x}|\mu, f, \phi) \quad (1)$$

where $\mathbf{p} = [\alpha, \mu, \sigma, \lambda]$ and $\mathcal{N}(\mathbf{x}|\mu, \sigma)$ is the Gaussian function given by

$$\mathcal{N}(\mathbf{x}|\mu, \sigma) = \exp\left(-\frac{(\mathbf{x} - \mu)^2}{2\sigma^2}\right) \quad (2)$$

with neglected normalization. The exponentially-modified term is modeled by

$$\Phi(\mathbf{x}|\lambda, \mu, \sigma) = \left(1 + \operatorname{erf}\left(\lambda \frac{\mathbf{x} - \mu}{\sigma\sqrt{2}}\right)\right) \quad (3)$$

and finally the oscillating term writes

$$A(\mathbf{x}|\mu, f, \phi) = \cos(2\pi f(\mathbf{x} - \mu) + \phi) \quad (4)$$

with frequency f and phase ϕ . Putting all terms together, the EMG writes

$$m(\mathbf{p}; \mathbf{x}) = \alpha \exp\left(-\frac{(\mathbf{x} - \mu)^2}{2\sigma^2}\right) \left(1 + \operatorname{erf}\left(\lambda \frac{\mathbf{x} - \mu}{\sigma\sqrt{2}}\right)\right) \cos(2\pi f(\mathbf{x} - \mu) + \phi) \quad (5)$$

Now we introduce an EMG mixture model by

$$M(\mathbf{P}; \mathbf{x}) = \sum_{k=1}^K m(\mathbf{p}_k; \mathbf{x}) \quad (6)$$

with components $k = \{1, 2, \dots, K\}$. For minimization, the loss function writes

$$L(\mathbf{P}) = (y - M(\mathbf{P}; \mathbf{x}))^2 \quad (7)$$

where y represents the measurement data suffering from noise.

$$\mathbf{P}^* = \arg \min_{\mathbf{P}} L(\mathbf{P}) \quad (8)$$

2 Analytical Derivative

$$\frac{\partial L(\mathbf{P})}{\partial \mathbf{P}} = \frac{\partial (y - M(\mathbf{P}; \mathbf{x}))^2}{\partial \mathbf{P}} \quad (9)$$

which becomes

$$\frac{\partial L(\mathbf{P})}{\partial \mathbf{P}} = 2(y - M(\mathbf{P}; \mathbf{x})) \frac{\partial (y - M(\mathbf{P}; \mathbf{x}))}{\partial \mathbf{P}} \quad (10)$$

after employing the chain rule.

$$\frac{\partial (y - M(\mathbf{P}; \mathbf{x}))}{\partial \mathbf{P}} = \frac{\partial y}{\partial \mathbf{P}} - \frac{\partial \left(\sum_k^K m(\mathbf{p}_k, \mathbf{x}) \right)}{\partial \mathbf{P}} = - \frac{\partial m(\mathbf{p}_k, \mathbf{x})}{\partial \mathbf{P}} \quad (11)$$

where we exploited that only the k -th mixture component depends on \mathbf{P}

2.1 Partial derivative w.r.t. μ

$$\frac{\partial m(\mathbf{p}, \mathbf{x})}{\partial \mu} = \frac{\partial}{\partial \mu} (\alpha \mathcal{N}(\mathbf{x}|\mu, \sigma) \Phi(\mathbf{x}|\lambda, \mu, \sigma) A(\mathbf{x}|\mu, f, \phi)) \quad (12)$$

which becomes

$$\frac{\partial m(\mathbf{p}, \mathbf{x})}{\partial \mu} = \alpha \left(\Phi(\mathbf{x}|\lambda, \mu, \sigma) A(\mathbf{x}|\mu, f, \phi) \frac{\partial \mathcal{N}(\mathbf{x}|\mu, \sigma)}{\partial \mu} \right. \quad (13)$$

$$\left. + \mathcal{N}(\mathbf{x}|\mu, \sigma) A(\mathbf{x}|\mu, f, \phi) \frac{\partial \Phi(\mathbf{x}|\lambda, \mu, \sigma)}{\partial \mu} \right. \quad (14)$$

$$\left. + \mathcal{N}(\mathbf{x}|\mu, \sigma) \Phi(\mathbf{x}|\lambda, \mu, \sigma) \frac{\partial A(\mathbf{x}|\mu, f, \phi)}{\partial \mu} \right) \quad (15)$$

after applying the product rule.

$$\frac{\partial \mathcal{N}(\mathbf{x}|\mu, \sigma)}{\partial \mu} = \frac{\partial}{\partial \mu} \exp \left(-\frac{(\mathbf{x} - \mu)^2}{2\sigma^2} \right) \quad (16)$$

$$\frac{\partial \mathcal{N}(\mathbf{x}|\mu, \sigma)}{\partial \mu} = \frac{\mathbf{x} - \mu}{\sigma^2} \exp \left(-\frac{(\mathbf{x} - \mu)^2}{2\sigma^2} \right) \quad (17)$$

$$\frac{\partial \Phi(\mathbf{x}|\lambda, \mu, \sigma)}{\partial \mu} = \frac{\partial}{\partial \mu} \left(1 + \operatorname{erf} \left(\lambda \frac{\mathbf{x} - \mu}{\sigma \sqrt{2}} \right) \right) \quad (18)$$

$$\frac{\partial \Phi(\mathbf{x}|\lambda, \mu, \sigma)}{\partial \mu} = \frac{\partial}{\partial \mu} \left(1 + \frac{2}{\sqrt{\pi}} \int_0^{\lambda \frac{\mathbf{x} - \mu}{\sigma \sqrt{2}}} \exp(-t^2) dt \right) \quad (19)$$

$$\frac{\partial \Phi(\mathbf{x}|\lambda, \mu, \sigma)}{\partial \mu} = \frac{2}{\sqrt{\pi}} \exp \left(-\lambda^2 \frac{(\mathbf{x} - \mu)^2}{2\sigma^2} \right) \left(-\frac{\lambda}{\sigma \sqrt{2}} \right) \quad (20)$$

$$\frac{\partial \Phi(\mathbf{x}|\lambda, \mu, \sigma)}{\partial \mu} = -\frac{2}{\sqrt{2\pi}} \frac{\lambda}{\sigma} \exp \left(-\lambda^2 \frac{(\mathbf{x} - \mu)^2}{2\sigma^2} \right) \quad (21)$$

which can be simplified with $\sqrt{\frac{2}{\pi}} = \frac{2}{\sqrt{2\pi}}$. Differentiating the oscillating term w.r.t. μ writes

$$\frac{\partial A(\mathbf{x}|\mu, f, \phi)}{\partial \mu} = \frac{\partial}{\partial \mu} \cos(2\pi f(\mathbf{x} - \mu) + \phi) \quad (22)$$

so that

$$\frac{\partial A(\mathbf{x}|\mu, f, \phi)}{\partial \mu} = 2\pi f \sin(2\pi f(\mathbf{x} - \mu) + \phi) \quad (23)$$

2.2 Partial derivative w.r.t. σ

$$\frac{\partial m(\mathbf{p}, \mathbf{x})}{\partial \sigma} = \frac{\partial}{\partial \sigma} (\alpha \mathcal{N}(\mathbf{x}|\mu, \sigma) \Phi(\mathbf{x}|\lambda, \mu, \sigma) A(\mathbf{x}|\mu, f, \phi)) \quad (24)$$

which becomes

$$\frac{\partial m(\mathbf{p}, \mathbf{x})}{\partial \sigma} = \alpha \left(\Phi(\mathbf{x}|\lambda, \mu, \sigma) A(\mathbf{x}|\mu, f, \phi) \frac{\partial \mathcal{N}(\mathbf{x}|\mu, \sigma)}{\partial \sigma} \right. \quad (25)$$

$$\left. + \mathcal{N}(\mathbf{x}|\mu, \sigma) A(\mathbf{x}|\mu, f, \phi) \frac{\partial \Phi(\mathbf{x}|\lambda, \mu, \sigma)}{\partial \sigma} \right. \quad (26)$$

$$\left. + \mathcal{N}(\mathbf{x}|\mu, \sigma) \Phi(\mathbf{x}|\lambda, \mu, \sigma) \frac{\partial A(\mathbf{x}|\mu, f, \phi)}{\partial \sigma} \right) \quad (27)$$

after applying the product rule.

$$\frac{\partial \mathcal{N}(\mathbf{x}|\mu, \sigma)}{\partial \sigma} = \frac{(\mathbf{x} - \mu)^2}{\sigma^3} \exp \left(-\frac{(\mathbf{x} - \mu)^2}{2\sigma^2} \right) \quad (28)$$

$$\frac{\partial \Phi(\mathbf{x}|\lambda, \mu, \sigma)}{\partial \sigma} = -\frac{2}{\sqrt{2\pi}} \frac{\lambda(\mathbf{x} - \mu)}{\sigma^2} \exp\left(-\lambda^2 \frac{(\mathbf{x} - \mu)^2}{2\sigma^2}\right) \quad (29)$$

which can be simplified with $\sqrt{\frac{2}{\pi}} = \frac{2}{\sqrt{2\pi}}$. Differentiating the oscillating term w.r.t. σ writes

$$\frac{\partial A(\mathbf{x}|\mu, f, \phi)}{\partial \sigma} = \frac{\partial}{\partial \sigma} \cos(2\pi f(\mathbf{x} - \mu) + \phi) \quad (30)$$

so that

$$\frac{\partial A(\mathbf{x}|\mu, f, \phi)}{\partial \sigma} = 0 \quad (31)$$

2.3 Partial derivative w.r.t. λ

$$\frac{\partial m(\mathbf{p}, \mathbf{x})}{\partial \lambda} = \frac{\partial}{\partial \lambda} (\alpha \mathcal{N}(\mathbf{x}|\mu, \sigma) \Phi(\mathbf{x}|\lambda, \mu, \sigma) A(\mathbf{x}|\mu, f, \phi)) \quad (32)$$

which becomes

$$\frac{\partial m(\mathbf{p}, \mathbf{x})}{\partial \lambda} = \alpha \mathcal{N}(\mathbf{x}|\mu, \sigma) A(\mathbf{x}|\mu, f, \phi) \frac{\partial \Phi(\mathbf{x}|\lambda, \mu, \sigma)}{\partial \lambda} \quad (33)$$

$$\frac{\partial \Phi(\mathbf{x}|\lambda, \mu, \sigma)}{\partial \lambda} = \frac{2}{\sqrt{2\pi}} \frac{\mathbf{x} - \mu}{\sigma} \exp\left(-\lambda^2 \frac{(\mathbf{x} - \mu)^2}{2\sigma^2}\right) \quad (34)$$

which can be simplified with $\sqrt{\frac{2}{\pi}} = \frac{2}{\sqrt{2\pi}}$.

2.4 Partial derivative w.r.t. α

$$\frac{\partial m(\mathbf{p}, \mathbf{x})}{\partial \alpha} = \frac{\partial}{\partial \alpha} \alpha (\mathcal{N}(\mathbf{x}|\mu, \sigma) \Phi(\mathbf{x}|\lambda, \mu, \sigma) A(\mathbf{x}|\mu, f, \phi)) \quad (35)$$

which becomes

$$\frac{\partial m(\mathbf{p}, \mathbf{x})}{\partial \alpha} = \mathcal{N}(\mathbf{x}|\mu, \sigma) \Phi(\mathbf{x}|\lambda, \mu, \sigma) A(\mathbf{x}|\mu, f, \phi) \quad (36)$$

2.5 Partial derivative w.r.t. f

$$\frac{\partial m(\mathbf{p}, \mathbf{x})}{\partial f} = \frac{\partial}{\partial f} \alpha (\mathcal{N}(\mathbf{x}|\mu, \sigma) \Phi(\mathbf{x}|\lambda, \mu, \sigma) A(\mathbf{x}|\mu, f, \phi)) \quad (37)$$

which becomes

$$\frac{\partial m(\mathbf{p}, \mathbf{x})}{\partial f} = \alpha \left(\Phi(\mathbf{x}|\lambda, \mu, \sigma) A(\mathbf{x}|\mu, f, \phi) \frac{\partial \mathcal{N}(\mathbf{x}|\mu, \sigma)}{\partial f} \right. \quad (38)$$

$$\left. + \mathcal{N}(\mathbf{x}|\mu, \sigma) A(\mathbf{x}|\mu, f, \phi) \frac{\partial \Phi(\mathbf{x}|\lambda, \mu, \sigma)}{\partial f} \right. \quad (39)$$

$$\left. + \mathcal{N}(\mathbf{x}|\mu, \sigma) \Phi(\mathbf{x}|\lambda, \mu, \sigma) \frac{\partial A(\mathbf{x}|\mu, f, \phi)}{\partial f} \right) \quad (40)$$

Differentiating the oscillating term w.r.t. f writes

$$\frac{\partial A(\mathbf{x}|\mu, f, \phi)}{\partial \sigma} = \frac{\partial}{\partial \sigma} \cos(2\pi f(\mathbf{x} - \mu) + \phi) \quad (41)$$

so that

$$\frac{\partial A(\mathbf{x}|\mu, f, \phi)}{\partial f} = 2\pi(\mu - \mathbf{x}) \sin(2\pi f(\mathbf{x} - \mu) + \phi) \quad (42)$$

2.6 Partial derivative w.r.t. ϕ

$$\frac{\partial m(\mathbf{p}, \mathbf{x})}{\partial \phi} = \frac{\partial}{\partial \phi} \alpha (\mathcal{N}(\mathbf{x}|\mu, \sigma) \Phi(\mathbf{x}|\lambda, \mu, \sigma) A(\mathbf{x}|\mu, f, \phi)) \quad (43)$$

which becomes

$$\frac{\partial m(\mathbf{p}, \mathbf{x})}{\partial \phi} = \alpha \left(\Phi(\mathbf{x}|\lambda, \mu, \sigma) A(\mathbf{x}|\mu, f, \phi) \frac{\partial \mathcal{N}(\mathbf{x}|\mu, \sigma)}{\partial \phi} \right. \quad (44)$$

$$\left. + \mathcal{N}(\mathbf{x}|\mu, \sigma) A(\mathbf{x}|\mu, f, \phi) \frac{\partial \Phi(\mathbf{x}|\lambda, \mu, \sigma)}{\partial \phi} \right. \quad (45)$$

$$\left. + \mathcal{N}(\mathbf{x}|\mu, \sigma) \Phi(\mathbf{x}|\lambda, \mu, \sigma) \frac{\partial A(\mathbf{x}|\mu, f, \phi)}{\partial \phi} \right) \quad (46)$$

Differentiating the oscillating term w.r.t. ϕ writes

$$\frac{\partial A(\mathbf{x}|\mu, f, \phi)}{\partial \phi} = \frac{\partial}{\partial \phi} \cos(2\pi f(\mathbf{x} - \mu) + \phi) \quad (47)$$

so that

$$\frac{\partial A(\mathbf{x}|\mu, f, \phi)}{\partial \phi} = -\sin(2\pi f(\mathbf{x} - \mu) + \phi) \quad (48)$$

3 Jacobian Matrix

The Jacobian matrix $\mathbf{J} \in \mathbb{R}^{N \times P}$ with N samples and P variables writes

$$\mathbf{J} = \gamma \begin{bmatrix} \frac{\partial m(\mathbf{p}_k, x_0)}{\partial \alpha} & \frac{\partial m(\mathbf{p}_k, x_0)}{\partial \mu} & \frac{\partial m(\mathbf{p}_k, x_0)}{\partial \sigma} & \frac{\partial m(\mathbf{p}_k, x_0)}{\partial \lambda} & \frac{\partial m(\mathbf{p}_k, x_0)}{\partial f} & \frac{\partial m(\mathbf{p}_k, x_0)}{\partial \phi} \\ \frac{\partial m(\mathbf{p}_k, x_1)}{\partial \alpha} & \frac{\partial m(\mathbf{p}_k, x_1)}{\partial \mu} & \frac{\partial m(\mathbf{p}_k, x_1)}{\partial \sigma} & \frac{\partial m(\mathbf{p}_k, x_1)}{\partial \lambda} & \frac{\partial m(\mathbf{p}_k, x_1)}{\partial f} & \frac{\partial m(\mathbf{p}_k, x_1)}{\partial \phi} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial m(\mathbf{p}_k, \mathbf{x})}{\partial \alpha} & \frac{\partial m(\mathbf{p}_k, \mathbf{x})}{\partial \mu} & \frac{\partial m(\mathbf{p}_k, \mathbf{x})}{\partial \sigma} & \frac{\partial m(\mathbf{p}_k, \mathbf{x})}{\partial \lambda} & \frac{\partial m(\mathbf{p}_k, \mathbf{x})}{\partial f} & \frac{\partial m(\mathbf{p}_k, \mathbf{x})}{\partial \phi} \end{bmatrix} \quad (49)$$

where the term $\gamma = -2(y - M(\mathbf{P}; \mathbf{x}))$ comes from the chain rule in Eq. (10). The Jacobian is used to update parameter estimates. This can be done in a Gauss-Newton update fashion as given by

$$\mathbf{p}_{k+1} = \mathbf{p}_k - \alpha (\mathbf{J}^\top \mathbf{J})^{-1} \mathbf{J}^\top \mathbf{x} \quad (50)$$

4 Combined partial derivatives

$$\frac{\partial L(\mathbf{P})}{\partial \mathbf{P}} = 2(M(\mathbf{P}; \mathbf{x}) - y) \frac{\partial m(\mathbf{p}_k, \mathbf{x})}{\partial \mathbf{P}} \quad (51)$$

4.1 Partial derivative w.r.t. μ

$$\frac{\partial m(\mathbf{p}, \mathbf{x})}{\partial \mu} = \alpha \left(\frac{\mathbf{x} - \mu}{\sigma^2} \mathcal{N}(\mathbf{x}|\mu, \sigma) \Phi(\mathbf{x}|\lambda, \mu, \sigma) A(\mathbf{x}|\mu, f, \phi) \right. \quad (52)$$

$$\left. - \frac{\exp\left(-\lambda^2 \frac{(\mathbf{x} - \mu)^2}{2\sigma^2}\right)}{\sigma \sqrt{2\pi}} \mathcal{N}(\mathbf{x}|\mu, \sigma) A(\mathbf{x}|\mu, f, \phi) \right. \quad (53)$$

$$\left. + 2\pi f \sin(2\pi f(\mathbf{x} - \mu) + \phi) \mathcal{N}(\mathbf{x}|\mu, \sigma) \Phi(\mathbf{x}|\lambda, \mu, \sigma) \right) \quad (54)$$

4.2 Partial derivative w.r.t. σ

$$\frac{\partial m(\mathbf{p}, \mathbf{x})}{\partial \sigma} = \alpha \mathcal{N}(\mathbf{x}|\mu, \sigma) A(\mathbf{x}|\mu, f, \phi) \left(\frac{(\mathbf{x} - \mu)^2}{\sigma^3} \Phi(\mathbf{x}|\lambda, \mu, \sigma) - \sqrt{\frac{2}{\pi}} \frac{\lambda(\mathbf{x} - \mu)}{\sigma^2} \exp\left(-\lambda^2 \frac{(\mathbf{x} - \mu)^2}{2\sigma^2}\right) \right) \quad (55)$$

4.3 Partial derivative w.r.t. λ

$$\frac{\partial m(\mathbf{p}, \mathbf{x})}{\partial \lambda} = -\alpha \mathcal{N}(\mathbf{x}|\mu, \sigma) A(\mathbf{x}|\mu, f, \phi) \sqrt{\frac{2}{\pi}} \frac{\mathbf{x} - \mu}{\sigma} \exp\left(-\lambda^2 \frac{(\mathbf{x} - \mu)^2}{2\sigma^2}\right) \quad (56)$$

4.4 Partial derivative w.r.t. α

$$\frac{\partial m(\mathbf{p}, \mathbf{x})}{\partial \alpha} = \mathcal{N}(\mathbf{x}|\mu, \sigma) \Phi(\mathbf{x}|\lambda, \mu, \sigma) A(\mathbf{x}|\mu, f, \phi) \quad (57)$$

4.5 Partial derivative w.r.t. f

$$\frac{\partial m(\mathbf{p}, \mathbf{x})}{\partial f} = \alpha \mathcal{N}(\mathbf{x}|\mu, \sigma) \Phi(\mathbf{x}|\lambda, \mu, \sigma) 2\pi (\mu - \mathbf{x}) \sin(2\pi f(\mathbf{x} - \mu) + \phi) \quad (58)$$

4.6 Partial derivative w.r.t. ϕ

$$\frac{\partial m(\mathbf{p}, \mathbf{x})}{\partial \phi} = -\alpha \mathcal{N}(\mathbf{x}|\mu, \sigma) \Phi(\mathbf{x}|\lambda, \mu, \sigma) \sin(2\pi f(\mathbf{x} - \mu) + \phi) \quad (59)$$