Analytical Derivation for Multimodal Exponentially Modified Gaussian Oscillators

Christopher Hahne

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This document elaborates on an analytical solution to the Multimodal Exponentially Modified Gaussian (MEMG) model using least-squares optimization.

1 Objective

Let the Exponentially Modified Gaussian (EMG) be

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

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

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

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

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

and finally the oscillating term writes

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

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

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

Now we introduce an EMG mixture model by

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

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

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

where y represents the measurement data suffering from noise.

$$\mathbf{P}^\star = \arg\min_{\mathbf{P}} L(\mathbf{P}) \tag{8}$$

2 Analytical Derivative

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

which becomes

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

after employing the chain rule.

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

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

2.1 Partial derivative w.r.t. μ

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

which becomes

$$\begin{aligned}
\frac{\partial m(\mathbf{p}, \mathbf{x})}{\partial \mu} = \alpha \Bigg(& \Phi(\mathbf{x}|\lambda, \mu, \sigma) \, A(\mathbf{x}|\mu, f, \phi) \frac{\partial \mathcal{N}(\mathbf{x}|\mu, \sigma)}{\partial \mu} && (13) \\
& + \mathcal{N}(\mathbf{x}|\mu, \sigma) \, A(\mathbf{x}|\mu, f, \phi) \frac{\partial \Phi(\mathbf{x}|\lambda, \mu, \sigma)}{\partial \mu} && (14) \\
& + \mathcal{N}(\mathbf{x}|\mu, \sigma) \, \Phi(\mathbf{x}|\lambda, \mu, \sigma) \frac{\partial A(\mathbf{x}|\mu, f, \phi)}{\partial \mu} \Bigg) && (15)
\end{aligned}$$

after applying the product rule.

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

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

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

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

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

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

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

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

so that

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

2.2 Partial derivative w.r.t. σ

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

which becomes

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

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

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

after applying the product rule.

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

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

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

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

so that

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

2.3 Partial derivative w.r.t. λ

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

which becomes

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

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

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

2.4 Partial derivative w.r.t. α

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

which becomes

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

2.5 Partial derivative w.r.t. f

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

which becomes

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

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

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

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

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

so that

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

2.6 Partial derivative w.r.t. ϕ

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

which becomes

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

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

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

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

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

so that

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

3 Jacobian Matrix

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

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

where the term $\gamma = -2\left(y - M\left(\mathbf{P}; \mathbf{x}\right)\right)$ 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

$$\mathbf{p}_{k+1} = \mathbf{p}_k - \alpha \left(\mathbf{J}^\intercal \mathbf{J}\right)^{-1} \mathbf{J}^\intercal \mathbf{x} \tag{50}$$

4 Combined partial derivatives

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

4.1 Partial derivative w.r.t. μ

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

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

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

4.2 Partial derivative w.r.t. σ

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

4.3 Partial derivative w.r.t. λ

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

4.4 Partial derivative w.r.t. α

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

4.5 Partial derivative w.r.t. f

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

4.6 Partial derivative w.r.t. ϕ

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