1 Derivations

1.1 Problem Definition

1.1.1 Bayesian Framework

We make a reasonable assumption that the measurement noise Σ_ν is zero-mean and normally distributed, with real and imaginary components jointly independent and of equal variance.

The uncertainty in model parameters is also assumed to be normally distributed. Means were selected to agree with literature values and variance to keep distribution values in a physically meaningful range. We assume that it is reasonable to treat these parameters as jointly independent, because each parameter belongs to a different tissue type.

$$\theta \sim \mathcal{N}\left(\boldsymbol{\mu}_\theta, \boldsymbol{\Sigma}_\theta\right) = \prod_{i=1}^{N} \mathcal{N}\left(\mu_{\theta_i}, \sigma_{\theta_i}\right)$$

$$z \mid \theta \sim \mathcal{CN}\left(\mathcal{G}\left(\theta\right), \boldsymbol{\Sigma}_\nu\right) = \mathcal{N}\left(\mathcal{G}_r\left(\theta\right), \sigma_\nu\right)\mathcal{N}\left(\mathcal{G}_i\left(\theta\right), \sigma_\nu\right)$$

1.1.2 Physics Model

The physics model used is the Pennes bioheat equation, a heat transfer equation in biological tissue. The source term models energy deposition by the laser fiber, and along with the thermal and optical properties of the involved tissues, solution of this equation yields tissue temperature.

$$\rho c \frac{\partial u}{\partial t} - \nabla \cdot \left(\lambda\left(u, \mathbf{x}\right) \nabla u\right) + \omega\left(u, \mathbf{x}\right) c_{blood}\left(u - u_a\right) = Q_{laser}\left(\mathbf{x}, t\right), \quad \forall \mathbf{x} \in \Omega \tag{1}$$

$$Q_{laser}\left(\mathbf{x}, t\right) = P\left(t\right) \mu^2 \frac{e^{-\mu\|\mathbf{x}-\mathbf{x}_0\|}}{4\pi\|\mathbf{x}-\mathbf{x}_0\|}$$

$$u\left(\mathbf{x}, 0\right) = u_0\left(\mathbf{x}\right), \quad \mathbf{x} \in \Omega$$

$$u\left(\mathbf{x}, t\right) = u_D\left(\mathbf{x}\right), \quad \mathbf{x} \in \partial\Omega_D$$

$$-\lambda\left(u, \mathbf{x}\right) \nabla \cdot u\left(\mathbf{x}, t\right) = g_N\left(\mathbf{x}\right), \quad \mathbf{x} \in \partial\Omega_N$$

$$-\lambda\left(u, \mathbf{x}\right) \nabla \cdot u\left(\mathbf{x}, t\right) = h\left(u - u_\infty\right), \quad \mathbf{x} \in \partial\Omega_c$$

$$\mu\left(\mathbf{x}\right) = \sum_{i=1}^{N} \mu_n U\left(\mathbf{x} - \Omega_n\right) \tag{2}$$

$$\bigcup_{i\,=n}^{N} \Omega_n = \Omega, \quad \Omega_n \cap \Omega_m = \varnothing$$

$$U\left(\mathbf{x} - \Omega_n\right) = \begin{cases} 1, & x \in \Omega_n \\ 0, & \text{otherwise} \end{cases}$$

1.1.3 Signal Model

$$z\left(\mu, \mathbf{k}\right) = \int_\Omega \left(M\left(\mathbf{x}\right) e^{-s\left(\mu, \mathbf{x}\right)}\right) e^{-2\pi \mathrm{i} \mathbf{k}\cdot\mathbf{x}} d\mathbf{x} + \nu, \quad \nu \sim \mathcal{N}\left(0, \sigma_\nu\right) \tag{3}$$

$$s\left(\mu, \mathbf{x}\right) = \frac{T_E}{T_2^*\left(\mathbf{x}\right)} + \mathrm{i}\left[2\pi\gamma\alpha B_0 T_E \Delta u\left(\mu, \mathbf{x}\right) + T_E \Delta\omega_0\left(\mathbf{x}\right)\right]$$

1.2 Gauss-Hermite Quadrature

Generally, a Gauss-Hermite quadrature rule of n points will produce the exact integral when $f(x)$ is a polynomial of degree $2n-1$ or less.

Gaussian quadrature:

$$\int_{-\infty}^{\infty} e^{-x^2} f(x)\, dx \approx \sum_{i=1}^{N} \omega_i f(x_i) \tag{4}$$

$$\omega_i = \frac{2^{n-1} n! \sqrt{\pi}}{n^2 \left[H_{n-1}(x_i)\right]^2}$$

where n is the number of sample points used, $H_n(x)$ is the physicists' Hermite polynomial, x_i are the roots of the Hermite polynomial, and ω_i are the associated Gauss-Hermite weights.

Substitution for normal distributions using Gauss-Hermite quadrature:

$$\mathrm{E}\left[h(y)\right] = \int_{-\infty}^{\infty} \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(y-\mu)^2}{2\sigma^2}\right) h(y)\, dy \tag{5}$$

h is some function of y, and random variable Y is normally distributed.

$$x = \frac{y-\mu}{\sqrt{2}\sigma} \Leftrightarrow y = \sqrt{2}\sigma x + \mu \tag{6}$$

$$\begin{aligned} \mathrm{E}\left[h(y)\right] &= \int_{-\infty}^{\infty} \frac{1}{\sqrt{\pi}} \exp\left(-x^2\right) h\left(\sqrt{2}\sigma x + \mu\right) dx \\ &\approx \frac{q}{\sqrt{\pi}} \sum_{i=1}^{N} \omega_i h\left(\sqrt{2}\sigma x_i + \mu\right) \end{aligned} \tag{7}$$

Multivariate Gauss-Hermite Quadrature:

$$\int_{-\infty}^{\infty} e^{-x^2} e^{-y^2} f(x,y)\, dxdy \approx \sum_{i=1}^{N_i} \sum_{j=1}^{N_j} \omega_i \theta_j f(x,y) \tag{8}$$

$$\omega_i = \frac{2^{n-1} n! \sqrt{\pi}}{n^2 \left[H_{n-1}(x_i)\right]^2}$$

1.3 Complex Normal Distribution Properties

The complex normal distribution is defined by the following equations for some k-dimensional random complex variable z:

$$p(z) = \pi^{-k} \left|\Gamma\right|^{-1/2} \left|P\right|^{-1/2} \exp\left[-\frac{1}{2} \begin{pmatrix} (\bar{z}-\bar{\mu})^T & (z-\mu)^T \end{pmatrix} \begin{pmatrix} \Gamma & C \\ \bar{C}^T & \bar{\Gamma} \end{pmatrix} \begin{pmatrix} z-\mu \\ \bar{z}-\bar{\mu} \end{pmatrix}\right] \tag{9}$$

$$
\begin{aligned}
P &= \bar{\Gamma} - RC \\
R &= \bar{C}^T \Gamma^{-1} \\
\Gamma &= V_{xx} + V_{yy} + \mathrm{i}\left(V_{yx} - V_{xy}\right) \\
C &= V_{xx} - V_{yy} + \mathrm{i}\left(V_{yx} + V_{xy}\right)
\end{aligned}
$$

For the conditional distribution $p\left(z \mid \theta\right)$, the mean is located by evaluating the signal model, so $\mu = \mathcal{G}\left(\theta\right)$. The real and imaginary components are also jointly independent ($V_{xy} = V_{yx} = 0$) with equal variance ($V_{xx} = V_{yy} = \sigma_\nu$), so $\Gamma = 2\sigma_\nu$, and $C = 0$.

$$
\begin{aligned}
p\left(z \mid \theta\right) &= \pi^{-k} \left|2\sigma_\nu\right|^{-1/2} \left|2\sigma_\nu\right|^{-1/2} \exp\left[-\frac{1}{2}\begin{pmatrix} \left(\bar{z}-\bar{\mu}\right)^T & \left(z-\mu\right)^T \end{pmatrix} \begin{pmatrix} 2\sigma_\nu & 0 \\ 0 & 2\sigma_\nu \end{pmatrix} \begin{pmatrix} z-\mu \\ \bar{z}-\bar{\mu} \end{pmatrix}\right] \\
&= \left(2\pi\sigma_\nu\right)^{-1} \exp\left[-\frac{1}{2}\left(\frac{\left(\bar{z}-\bar{\mu}\right)\left(z-\mu\right)}{2\sigma_\nu} + \frac{\left(z-\mu\right)\left(\bar{z}-\bar{\mu}\right)}{2\sigma_\nu}\right)\right] \\
&= \left(2\pi\sigma_\nu\right)^{-1} \exp\left(-\frac{z\bar{z} - \mu\bar{z} - z\bar{\mu} + \mu\bar{\mu}}{2\sigma_\nu}\right) \\
&= \left(2\pi\sigma_\nu\right)^{-1} \exp\left(-\frac{z_r^2 + z_i^2 - 2z_r\mu_r - 2z_i\mu_i + \mu_r^2 + \mu_i^2}{2\sigma_\nu}\right) \\
&= \left(2\pi\sigma_\nu\right)^{-1/2} \exp\left(-\frac{\left(z_r-\mu_r\right)^2}{2\sigma_\nu}\right) \left(2\pi\sigma_\nu\right)^{-1/2} \exp\left(-\frac{\left(z_i-\mu_i\right)^2}{2\sigma_\nu}\right) \\
&= p\left(z_r \mid \theta\right) p\left(z_i \mid \theta\right)
\end{aligned}
\tag{10}
$$

Hence, we can show that the conditional distribution $p\left(z \mid \theta\right)$ is separable into the product of the one-dimensional normal conditional distributions of its real and imaginary components.

1.4 Multivariate Normal Distribution Properties

Assume normal distribution for the model parameter, optical attenuation coefficient $\boldsymbol{\mu}$.

$$
p\left(\boldsymbol{\mu}\right) = \mathcal{N}\left(\mathbf{m}_\mu, \boldsymbol{\Sigma}_\mu\right) \tag{11}
$$

$$
\mathbf{m}_\mu = \begin{bmatrix} m_{\mu_1} \\ \vdots \\ m_{\mu_N} \end{bmatrix} \tag{12a}
$$

$$
\boldsymbol{\Sigma}_\mu = \begin{bmatrix} \sigma_{\mu_1} & 0 & \cdots & 0 & 0 \\ 0 & \sigma_{\mu_2} & 0 & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & 0 & \sigma_{\mu_{N-1}} & 0 \\ 0 & 0 & \cdots & 0 & \sigma_{\mu_N} \end{bmatrix} \tag{12b}
$$

Similarly, the various tissue types are independent, and the covariance matrix $\boldsymbol{\Sigma}_\mu$ is also diagonal.

$$
p\left(\boldsymbol{\mu}\right) = \mathcal{N}_{\boldsymbol{\mu}}\left(\mathbf{m}_\mu, \boldsymbol{\Sigma}_\mu\right) = \prod_{i=1}^{N} \mathcal{N}_{\mu_i}\left(m_{\mu_i}, \sigma_{\mu_i}\right) = \prod_{i=1}^{N} p\left(\mu_i\right) \tag{13}
$$

1.5 Quadrature Approximation to $p(z)$

The signal measurement probability distribution $p(\mathbf{z})$ can be approximated using Gauss-Hermite quadrature. The calculation is performed separately for the real and imaginary components, $p(z_r)$ and $p(z_i)$, because z_r and z_i are independent.

$$\begin{aligned} p(z_r) &= \int_{-\infty}^{\infty} p(z_r \mid \boldsymbol{\mu}) \prod_{n=1}^{N} p(\mu_n)\, d\boldsymbol{\mu} = \int_{-\infty}^{\infty} p(z_r \mid \boldsymbol{\mu}) \prod_{n=1}^{N} \frac{1}{\sqrt{2\pi}\sigma_{\mu_n}} \exp\left(-\frac{(\mu_n - m_{\mu_n})^2}{2\sigma_{\mu_n}^2}\right) d\boldsymbol{\mu} \\ &= \int_{-\infty}^{\infty} p(z_r \mid \boldsymbol{\mu}) \prod_{n=1}^{N} \frac{1}{\sqrt{\pi}} \exp\left(-x_n^2\right) d\mathbf{x} \approx \pi^{-N/2} \sum_{p=1}^{Q^N} \omega_p p\left(z_r \mid \boldsymbol{\mu}_p\right) \end{aligned} \tag{14}$$

Q=number of quadrature points; N=number of tissue types

$$\begin{aligned} & p(z_r \mid \boldsymbol{\mu}) = p(z_r \mid \mu_1, \ldots, \mu_N) \\ & p\left(z_r \mid \boldsymbol{\mu}_p\right) = p(z_r \mid \mu_{1,q}, \ldots, \mu_{N,q}) \\ & d\boldsymbol{\mu} = d\mu_1 \cdots d\mu_N \\ & \mu_{i,q} = \sqrt{2}\sigma_{\mu_i} x_{i,q} + m_{\mu_i} \\ & d\mu_{i,q} = \sqrt{2}\sigma_{\mu_i} dx_{i,q} \end{aligned}$$

An identical calculation for the imaginary component results in

$$p(z_i) \approx \pi^{-N/2} \sum_{i=1}^{N} \sum_{q=1}^{Q} \omega_{i,q} p\left(z_i \mid \boldsymbol{\mu}_p\right) \tag{15}$$

$$p\left(z_i \mid \boldsymbol{\mu}_p\right) = p(z_i \mid \mu_{1,q}, \ldots, \mu_{N,q})$$

$$\mu_{i,q} = \sqrt{2}\sigma_{\mu_i} x_{i,q} + m_{\mu_i}$$

1.6 Quadrature Approximation to Entropy $H(z)$

Differential entropy:

$$
\begin{aligned}
H(z) &= -\int\limits_z p(z)\ln\left[p(z)\right]dz \\
&\approx -\int\limits_z \ln\left[p(z)\right]\pi^{-N/2}\sum_{i=1}^{Q^N}\omega_i p(z\mid\theta_i)\,dz \\
&= -\pi^{-N/2}\sum_{i=1}^{Q^N}\omega_i\int\limits_z \ln\left[p(z)\right]p(z\mid\theta_i)\,dz \\
&= -\pi^{-N/2}\sum_{i=1}^{Q^N}\omega_i\int\limits_{z_r}\int\limits_{z_i}\ln\left[\pi^{-N/2}\sum_{k=1}^{Q^N}\omega_k p(z_r\mid\theta_k)\,p(z_i\mid\theta_k)\right]p(z_r\mid\theta_i)\,p(z_i\mid\theta_i)\,dz_r dz_i \\
&= -\pi^{-N/2}\sum_{i=1}^{Q^N}\omega_i\int\limits_{z_r}\int\limits_{z_i}\left(2\pi\sigma_\nu^2\right)^{-1}\exp\left(-\frac{\left(z_r-\mathcal{G}_r(\theta_i)\right)^2}{2\sigma_\nu^2}\right)\exp\left(-\frac{\left(z_i-\mathcal{G}_i(\theta_i)\right)^2}{2\sigma_\nu^2}\right) \\
&\quad\cdot\ln\left[\pi^{-N/2}\sum_{k=1}^{Q^N}\omega_k p(z_r\mid\theta_k)\,p(z_i\mid\theta_k)\right]dz_r dz_i \\
&= -\pi^{-N/2}\sum_{i=1}^{Q^N}\omega_i\int\limits_{x_r}\int\limits_{x_i}\pi^{-1}\exp\left(-x_r(\theta_i)\right)\exp\left(-x_i(\theta_i)\right) \\
&\quad\cdot\ln\left[\pi^{-N/2}\sum_{k=1}^{Q^N}\omega_k p\left(\sqrt{2}\sigma_\nu x_r+\mathcal{G}(\theta_i)\mid\theta_k\right)p\left(\sqrt{2}\sigma_\nu x_i+\mathcal{G}(\theta_i)\mid\theta_k\right)\right]dx_r dx_i \\
&\approx -\pi^{-N/2-1}\sum_{i=1}^{Q^N}\omega_i\sum_{j=1}^{Q_z^2}\omega_j\ln\left[\pi^{-N/2}\sum_{k=1}^{Q^N}\omega_k p(z_{r,j}\mid\theta_k)\,p(z_{i,j}\mid\theta_k)\right] \\
&= -\pi^{-N/2}\sum_{i=1}^{Q^N}\omega_i\sum_{j=1}^{Q_z^2}\omega_j\ln\left[\pi^{-N/2}\sum_{k=1}^{Q^N}\omega_k\left(2\pi\sigma_\nu\right)^{-1}\exp\left(-\frac{\left(z_{r,j}-\mathcal{G}_r(\theta_k)\right)^2}{2\sigma_\nu^2}\right)\exp\left(-\frac{\left(z_{i,j}-\mathcal{G}_i(\theta_k)\right)^2}{2\sigma_\nu^2}\right)\right] \\
&= -\pi^{-N/2}\sum_{i=1}^{Q^N}\omega_i\sum_{j=1}^{Q_z^2}\omega_j\ln\left[\pi^{-N/2}\sum_{k=1}^{Q^N}\omega_k\left(2\pi\sigma_\nu\right)^{-1}\exp\left(-\frac{\left(\sqrt{2}\sigma_\nu x_{r,j}+\mathcal{G}_r(\theta_i)-\mathcal{G}_r(\theta_k)\right)^2}{2\sigma_\nu^2}\right)\right. \\
&\left.\cdot\exp\left(-\frac{\left(\sqrt{2}\sigma_\nu x_{i,j}+\mathcal{G}_r(\theta_i)-\mathcal{G}_i(\theta_k)\right)^2}{2\sigma_\nu^2}\right)\right]
\end{aligned}
\tag{16}
$$

$$
\begin{aligned}
x_r &= \frac{z_r-\mathcal{G}_r(\theta_i)}{\sqrt{2}\sigma_\nu} \\
z_r &= \sqrt{2}\sigma_\nu x_r+\mathcal{G}_r(\theta_i) \\
dx_r &= \frac{dz_r}{\sqrt{2}\sigma_\nu} \\
dz_r &= \sqrt{2}\sigma_\nu dx_r
\end{aligned}
$$