

# Channel-Aware Laplace Approximation for the Posterior over $p$

This note collects the derivations for a channel-aware Laplace approximation of the posterior over the macroscopic occupancy vector  $p$  of an ensemble of Markov channels, based on a single interval-averaged current measurement.

The main goals are:

- to obtain an explicit formula for the *Gaussian (Laplace) posterior covariance*  $\Sigma_{\text{post}}$  in terms of the prior covariance  $\Sigma_p$  and a rank-1 update defined by the measurement;
- to write the *mean update* in a form that does not involve any explicit inverse of the (singular) prior covariance;
- to emphasise that the posterior mean used in practice is the *MAP estimate* obtained by Newton iteration, and the covariance is the *Laplace covariance* given by the curvature at the MAP.

Throughout, we keep the dependence of all intermediate objects on  $p$  explicit:  $\delta(p)$ ,  $V(p)$ ,  $v(p)$ , etc. Whenever we drop the argument and write  $\delta$ ,  $V$ ,  $v$ , they are implicitly evaluated at the current expansion point (either a fixed  $p_0$ , or the current iterate  $p^{(k)}$  in Newton's method).

**Coordinates, simplex and singular covariance.** The macroscopic occupancy vector  $p$  lives on the simplex  $\{p \in \mathbb{R}^{1 \times d} : p_i \geq 0, \sum_i p_i = 1\}$ , a  $(d-1)$ -dimensional manifold embedded in  $\mathbb{R}^{1 \times d}$ . The prior covariance  $\Sigma_p$  is therefore singular as a  $d \times d$  matrix in ambient coordinates. Formally, one can view  $\Sigma_p^{-1}$  as the inverse on the  $(d-1)$ -dimensional tangent subspace or as a pseudo-inverse, but *in all final expressions we use in implementation,  $\Sigma_p^{-1}$  cancels algebraically*. We never need to numerically invert a singular covariance.

## 1. Setup and Notation

We consider:

- A macroscopic occupancy vector

$$p \in \mathbb{R}^{1 \times d},$$

a row vector of state probabilities.

- A per-state conductance vector

$$\gamma \in \mathbb{R}^{d \times 1},$$

a column vector.

- A per-state intrinsic-variance vector

$$\sigma^2 \in \mathbb{R}^{d \times 1}.$$

The prior over  $p$  (restricted to the simplex) is Gaussian:

$$p \sim \mathcal{N}(\mu, \Sigma_p),$$

where  $\mu \in \mathbb{R}^{1 \times d}$  is the prior mean and  $\Sigma_p \in \mathbb{R}^{d \times d}$  is the prior covariance. As noted above,  $\Sigma_p$  is singular in the ambient coordinates.

We observe a scalar interval-averaged current  $y$ :

$$y \approx N_{\text{ch}}(p \cdot \gamma) + \text{noise},$$

with  $N_{\text{ch}}$  channels and:

- extrinsic (measurement) noise variance  $\epsilon^2$ ;
- intrinsic ensemble variance  $N_{\text{ch}}(p \cdot \sigma^2)$  arising from channel stochasticity.

Given a candidate state  $p$ , define

$$\begin{aligned} \delta(p) &= y - N_{\text{ch}}(p \cdot \gamma), \\ V(p) &= \epsilon^2 + N_{\text{ch}}(p \cdot \sigma^2), \end{aligned}$$

and the *tilted* vector

$$v(p) = \gamma + \frac{\delta(p)}{V(p)} \sigma^2 \in \mathbb{R}^{d \times 1}.$$

We work with an energy function  $E(p)$  proportional to the negative log-posterior,

$$p(p \mid y) \propto \exp\left(-\frac{1}{2}E(p)\right).$$

We will denote:

- $\mathbf{g}(p) = \nabla E(p)$ , a *row* vector in  $\mathbb{R}^{1 \times d}$ ;
- $\mathbf{H}(p) = \nabla^2 E(p)$ , a  $d \times d$  Hessian.

## 2. Laplace Approximation Around an Expansion Point

We approximate the posterior around an expansion point  $p_0$  via a second-order Taylor expansion:

$$E(p) \approx E(p_0) + (p - p_0) \mathbf{g}_0^\top + \frac{1}{2}(p - p_0) \mathbf{H}_0 (p - p_0)^\top,$$

with

$$\mathbf{g}_0 = \nabla E(p_0), \quad \mathbf{H}_0 = \nabla^2 E(p)|_{p=p_0}.$$

Plugging this into

$$p(p \mid y) \propto \exp\left(-\frac{1}{2}E(p)\right)$$

gives a Gaussian approximation

$$p(p \mid y) \approx \mathcal{N}(p_{\text{post}}, \Sigma_{\text{post}}),$$

with

$$\Sigma_{\text{post}} \approx 2 \mathbf{H}_0^{-1},$$

$$p_{\text{post}} \approx p_0 - \mathbf{g}_0 \mathbf{H}_0^{-1} = p_0 - \frac{1}{2} \mathbf{g}_0 \Sigma_{\text{post}}.$$

Conceptually, the Laplace covariance is the inverse curvature at the chosen expansion point, and the mean is the Newton step from  $p_0$ . In practice, we will:

- use a special rank-1 structure of  $\mathbf{H}_0$  to obtain a closed-form  $\Sigma_{\text{post}}$  in terms of  $\Sigma_p$ ;
- eliminate any explicit  $\Sigma_p^{-1}$  from the mean update;
- iterate the Newton step until convergence to obtain the MAP.

### 3. Energy, Gradient and Hessian as Functions of $p$

We decompose the energy into likelihood and prior terms:

$$E(p) = M(p) + P(p),$$

with

$$M(p) = \frac{\delta(p)^2}{V(p)},$$

$$P(p) = (p - \mu) (N_{\text{ch}} \Sigma_p^{-1}) (p - \mu)^\top.$$

Here

$$\delta(p) = y - N_{\text{ch}}(p \cdot \gamma), \quad V(p) = \epsilon^2 + N_{\text{ch}}(p \cdot \sigma^2).$$

The full gradient and Hessian, derived in detail in Section 7, can be compactly written as:

$$\mathbf{g}(p) = 2N_{\text{ch}}(p - \mu)\Sigma_p^{-1} - N_{\text{ch}} \left[ \frac{2\delta(p)}{V(p)} \gamma^\top + \frac{\delta(p)^2}{V(p)^2} (\sigma^2)^\top \right],$$

and

$$\mathbf{H}(p) = 2N_{\text{ch}} \left[ \Sigma_p^{-1} + \frac{N_{\text{ch}}}{V(p)} v(p) v(p)^\top \right],$$

where

$$v(p) = \gamma + \frac{\delta(p)}{V(p)} \sigma^2.$$

These expressions are valid for all  $p$  on the simplex. They show explicitly that  $\delta$ ,  $V$  and  $v$  are functions of  $p$ .

### 4. Rank-1 Structure and Closed-Form Covariance

The key structural observation is that the Hessian is a rank-1 update of the prior precision:

$$\mathbf{H}(p) = 2N_{\text{ch}} \left[ \Sigma_p^{-1} + \frac{N_{\text{ch}}}{V(p)} v(p) v(p)^\top \right].$$

Define

$$u(p) = \sqrt{\frac{N_{\text{ch}}}{V(p)}} v(p), \quad \Rightarrow \quad u(p) u(p)^\top = \frac{N_{\text{ch}}}{V(p)} v(p) v(p)^\top.$$

Then

$$\mathbf{H}(p) = 2N_{\text{ch}} (\Sigma_p^{-1} + u(p) u(p)^\top).$$

#### 4.1 Sherman–Morrison Formula

Formally, for an invertible matrix  $A$  and a rank-1 update  $uu^\top$ , the Sherman–Morrison formula says

$$(A + uu^\top)^{-1} = A^{-1} - \frac{A^{-1}uu^\top A^{-1}}{1 + u^\top A^{-1}u}.$$

We apply this with  $A = \Sigma_p^{-1}$  and  $u = u(p_0)$  at the expansion point  $p_0$ . On the tangent subspace of the simplex,  $\Sigma_p$  has an inverse; at the algebraic level we write  $A^{-1} = \Sigma_p$  and obtain

$$(\Sigma_p^{-1} + uu^\top)^{-1} = \Sigma_p - \frac{\Sigma_p uu^\top \Sigma_p}{1 + u^\top \Sigma_p u}.$$

Since

$$\mathbf{H}_0 = 2N_{\text{ch}}(\Sigma_p^{-1} + uu^\top),$$

we get

$$\mathbf{H}_0^{-1} = \frac{1}{2N_{\text{ch}}} \left[ \Sigma_p - \frac{\Sigma_p uu^\top \Sigma_p}{1 + u^\top \Sigma_p u} \right].$$

The Laplace covariance at  $p_0$  is

$$\Sigma_{\text{post}} = 2\mathbf{H}_0^{-1} = \frac{1}{N_{\text{ch}}} \left[ \Sigma_p - \frac{\Sigma_p uu^\top \Sigma_p}{1 + u^\top \Sigma_p u} \right].$$

#### 4.2 Expressing Everything in Terms of $v(p_0)$

At  $p_0$  we have  $u = \sqrt{\frac{N_{\text{ch}}}{V}} v$  with  $V = V(p_0)$  and  $v = v(p_0)$ , so:

$$uu^\top = \frac{N_{\text{ch}}}{V} vv^\top,$$

and we define

$$s = v^\top \Sigma_p v.$$

Then:

$$\begin{aligned} \Sigma_p uu^\top \Sigma_p &= \Sigma_p \left( \frac{N_{\text{ch}}}{V} vv^\top \right) \Sigma_p = \frac{N_{\text{ch}}}{V} \Sigma_p vv^\top \Sigma_p, \\ 1 + u^\top \Sigma_p u &= 1 + \frac{N_{\text{ch}}}{V} v^\top \Sigma_p v = 1 + \frac{N_{\text{ch}}}{V} s = \frac{V + N_{\text{ch}} s}{V}. \end{aligned}$$

Substituting:

$$\Sigma_{\text{post}} = \frac{1}{N_{\text{ch}}} \left[ \Sigma_p - \frac{\frac{N_{\text{ch}}}{V} \Sigma_p v v^\top \Sigma_p}{\frac{V + N_{\text{ch}} s}{V}} \right] = \frac{1}{N_{\text{ch}}} \left[ \Sigma_p - \frac{N_{\text{ch}}}{V + N_{\text{ch}} s} \Sigma_p v v^\top \Sigma_p \right].$$

Thus we obtain the closed-form Laplace covariance:

$$\Sigma_{\text{post}}(p_0) = \frac{1}{N_{\text{ch}}} \Sigma_p - \frac{1}{V(p_0) + N_{\text{ch}} s(p_0)} \Sigma_p v(p_0) v(p_0)^\top \Sigma_p$$

with  $s(p_0) = v(p_0)^\top \Sigma_p v(p_0)$ .

**Singular covariance and implementation.** Note that:

- The derivation uses  $\Sigma_p^{-1}$  only as a formal device on the intrinsic  $(d-1)$ -dimensional subspace.
- The final expression for  $\Sigma_{\text{post}}$  involves only  $\Sigma_p$ ,  $v$  and  $s$ ; no explicit inverse of  $\Sigma_p$  appears.
- This formula remains valid even when  $\Sigma_p$  is singular in ambient coordinates, so it is suitable for direct implementation.

## 5. Mean Update and Elimination of $\Sigma_p^{-1}$

The Laplace mean at  $p_0$  is

$$p_{\text{post}} \approx p_0 - \mathbf{g}_0 \mathbf{H}_0^{-1} = p_0 - \frac{1}{2} \mathbf{g}_0 \Sigma_{\text{post}},$$

with

$$\mathbf{g}_0 = 2N_{\text{ch}}(p_0 - \mu) \Sigma_p^{-1} - N_{\text{ch}} \left[ \frac{2\delta}{V} \gamma^\top + \frac{\delta^2}{V^2} (\sigma^2)^\top \right],$$

where  $\delta = \delta(p_0)$  and  $V = V(p_0)$ .

Introduce

$$\Delta p = p_0 - \mu,$$

and rewrite:

$$\mathbf{g}_0 = 2N_{\text{ch}} \Delta p \Sigma_p^{-1} - N_{\text{ch}} \left[ \frac{2\delta}{V} \gamma^\top + \frac{\delta^2}{V^2} (\sigma^2)^\top \right].$$

Then

$$p_{\text{post}} = p_0 - \frac{1}{2} \mathbf{g}_0^\top \Sigma_{\text{post}} = p_0 - N_{\text{ch}} \Delta p \Sigma_p^{-1} \Sigma_{\text{post}} + \frac{N_{\text{ch}}}{2} \left[ \frac{2\delta}{V} \gamma^\top + \frac{\delta^2}{V^2} (\sigma^2)^\top \right] \Sigma_{\text{post}}.$$

Equivalently,

$$p_{\text{post}} = p_0 - N_{\text{ch}} \Delta p \Sigma_p^{-1} \Sigma_{\text{post}} + \frac{N_{\text{ch}} \delta}{V} \gamma^\top \Sigma_{\text{post}} + \frac{N_{\text{ch}} \delta^2}{2V^2} (\sigma^2)^\top \Sigma_{\text{post}}.$$

### 5.1 Eliminating $\Sigma_p^{-1}$ Using $\Sigma_{\text{post}}$

We now use the explicit expression for

$$\Sigma_{\text{post}} = \frac{1}{N_{\text{ch}}} \Sigma_p - \frac{1}{V + N_{\text{ch}} s} \Sigma_p v v^\top \Sigma_p$$

to compute  $\Sigma_p^{-1} \Sigma_{\text{post}}$  and thereby eliminate  $\Sigma_p^{-1}$  from the mean.

For notational compactness in this subsection, write  $N = N_{\text{ch}}$ , remembering they are the same quantity.

First:

$$\begin{aligned} \Sigma_p^{-1} \Sigma_{\text{post}} &= \Sigma_p^{-1} \left( \frac{1}{N} \Sigma_p - \frac{1}{V + N s} \Sigma_p v v^\top \Sigma_p \right) \\ &= \frac{1}{N} \underbrace{\Sigma_p^{-1} \Sigma_p}_I - \frac{1}{V + N s} v v^\top \Sigma_p \\ &= \frac{1}{N} I - \frac{1}{V + N s} v v^\top \Sigma_p. \end{aligned}$$

Therefore:

$$N \Delta p \Sigma_p^{-1} \Sigma_{\text{post}} = \Delta p - \frac{N}{V + N s} \Delta p v v^\top \Sigma_p.$$

Substituting into the expression for  $p_{\text{post}}$ :

$$\begin{aligned} p_{\text{post}} &= p_0 - \left[ \Delta p - \frac{N}{V + N s} \Delta p v v^\top \Sigma_p \right] + \frac{N \delta}{V} \gamma^\top \Sigma_{\text{post}} + \frac{N \delta^2}{2V^2} (\sigma^2)^\top \Sigma_{\text{post}} \\ &= (p_0 - \Delta p) + \frac{N}{V + N s} \Delta p v v^\top \Sigma_p + \frac{N \delta}{V} \gamma^\top \Sigma_{\text{post}} + \frac{N \delta^2}{2V^2} (\sigma^2)^\top \Sigma_{\text{post}}. \end{aligned}$$

Since  $p_0 - \Delta p = \mu$ , we obtain:

$$\begin{aligned} p_{\text{post}} &= \mu + \frac{N_{\text{ch}}}{V + N_{\text{ch}} s} (p_0 - \mu) v v^\top \Sigma_p \\ &\quad + \frac{N_{\text{ch}} \delta}{V} \gamma^\top \Sigma_{\text{post}} + \frac{N_{\text{ch}} \delta^2}{2V^2} (\sigma^2)^\top \Sigma_{\text{post}}. \end{aligned}$$

(2)

Here  $\Sigma_{\text{post}}$  is already expressed purely in terms of  $\Sigma_p$ ,  $v$ ,  $s$  and  $V$ . No explicit  $\Sigma_p^{-1}$  survives: it has been completely cancelled.

**Interpretation.**

- The first line in (2) pulls the mean back towards the prior mean  $\mu$ , modulated by the rank-1 direction  $vv^\top \Sigma_p$  and the competition between  $V$  and  $N_{\text{ch}}s$ .
- The second line captures the direct influence of the residual  $\delta$  through the conductance and intrinsic variance vectors  $(\gamma, \sigma^2)$ , weighted by the covariance  $\Sigma_{\text{post}}$ .
- Equation (2) is the general mean update that should be implemented numerically; it only requires multiplications by  $\Sigma_p$  and  $\Sigma_{\text{post}}$ , never their inverses.

**5.2 Special Case: Expansion at the Prior Mean  $p_0 = \mu$**

Choosing  $p_0 = \mu$  simplifies the expression significantly:

- $\Delta p = p_0 - \mu = 0$ ,
- the first line in (2) vanishes,
- the gradient at  $\mu$  reduces to

$$\mathbf{g}_0 = -N_{\text{ch}} \frac{\delta}{V} (\gamma^\top + v^\top),$$

so

$$p_{\text{post}} = \mu - \frac{1}{2} \mathbf{g}_0 \Sigma_{\text{post}} = \mu + \frac{N_{\text{ch}} \delta}{2V} (\gamma^\top + v^\top) \Sigma_{\text{post}}.$$

In this special case we obtain the concise one-step update:

$$p_{\text{post}} \approx \mu + \frac{N_{\text{ch}} \delta}{2V} (\gamma^\top + v^\top) \Sigma_{\text{post}},$$

with

- $\delta = y - N_{\text{ch}}(\mu \cdot \gamma)$ ,
- $V = \epsilon^2 + N_{\text{ch}}(\mu \cdot \sigma^2)$ ,
- $v = \gamma + \frac{\delta}{V} \sigma^2$ ,



- $\Sigma_{\text{post}}$  as in Section 4 with  $p_0 = \mu$ .

This corresponds to a single Newton step from the prior mean, with a Laplace covariance frozen at that expansion point.

## 6. Newton–MAP Scheme and MAP–Laplace Posterior

Up to now,  $p_0$  has been a generic expansion point. We now make explicit that:

- the posterior mean of interest is the *MAP*  $p^\star$ , i.e. the minimum of  $E(p)$ ;
- the covariance we associate with this mean is the *Laplace covariance*  $\Sigma_{\text{Lap}}$  given by the curvature at  $p^\star$ .

### 6.1 Defining the MAP

The posterior mode (MAP) is defined by

$$p^\star = \arg \min_p E(p)$$

subject to the simplex constraints  $p_i \geq 0$  and  $\sum_i p_i = 1$ . We seek this mode via Newton’s method applied to  $E(p)$ .

### 6.2 Newton Iteration

Let  $p^{(k)}$  denote the current iterate (row vector). One Newton step is:

$$p^{(k+1)} = p^{(k)} - \Delta p^{(k)}, \quad \mathbf{H}(p^{(k)}) \Delta p^{(k)\top} = \mathbf{g}(p^{(k)})^\top.$$

Algorithmically:

1. Initialise with a feasible point, typically  $p^{(0)} = \mu$ .
2. For  $k = 0, 1, 2, \dots$  until convergence:
  - (a) Compute  $\delta^{(k)} = \delta(p^{(k)})$ ,  $V^{(k)} = V(p^{(k)})$ ,  $v^{(k)} = v(p^{(k)})$ .
  - (b) Form  $\mathbf{g}^{(k)} = \mathbf{g}(p^{(k)})$  and  $\mathbf{H}^{(k)} = \mathbf{H}(p^{(k)})$  using the formulas in Section 3.

- (c) Compute the Laplace covariance  $\Sigma_{\text{post}}^{(k)}$  at  $p^{(k)}$  using the closed form in Section 4.
- (d) Update the mean using the general formula (2) with  $p_0 = p^{(k)}$  and  $\Sigma_{\text{post}} = \Sigma_{\text{post}}^{(k)}$ :

$$p^{(k+1)} = \mu + \frac{N_{\text{ch}}}{V^{(k)} + N_{\text{ch}} s^{(k)}} (p^{(k)} - \mu) v^{(k)} v^{(k)\top} \Sigma_p + \frac{N_{\text{ch}} \delta^{(k)}}{V^{(k)}} \gamma^\top \Sigma_{\text{post}}^{(k)} + \frac{N_{\text{ch}} \delta^{(k)2}}{2V^{(k)2}} (\sigma^2)^\top \Sigma_{\text{post}}^{(k)}.$$

Here  $s^{(k)} = v^{(k)\top} \Sigma_p v^{(k)}$ .

- (e) Optionally project  $p^{(k+1)}$  back onto the simplex (enforce  $p_i^{(k+1)} \geq 0$  and renormalise  $\sum_i p_i^{(k+1)} = 1$ ).

If we stop after a single iteration from  $p^{(0)} = \mu$ , we recover the one-step expression of Section 5.2. In general, Newton generates a sequence  $p^{(k)}$  converging to the MAP  $p^*$ , and we then set:

$$p_{\text{MAP}} = p^*.$$

### 6.3 MAP–Laplace Posterior

Once Newton has converged to  $p^*$ , we define the *MAP–Laplace posterior* as:

$$p \mid y \approx \mathcal{N}(p^*, \Sigma_{\text{Lap}}),$$

with covariance given by the inverse curvature at  $p^*$ :

$$\Sigma_{\text{Lap}} = \mathbf{H}(p^*)^{-1}.$$

Using the rank-1 structure, we compute  $\Sigma_{\text{Lap}}$  via the same closed form as  $\Sigma_{\text{post}}(p_0)$ , simply evaluated at  $p_0 = p^*$ :

$$\Sigma_{\text{Lap}} = \frac{1}{N_{\text{ch}}} \Sigma_p - \frac{1}{V(p^*) + N_{\text{ch}} s(p^*)} \Sigma_p v(p^*) v(p^*)^\top \Sigma_p,$$

with  $s(p^*) = v(p^*)^\top \Sigma_p v(p^*)$ .

Thus the computational recipe is:

- iterate Newton using (2) until convergence to  $p^*$ ;
- evaluate the rank-1 covariance formula at  $p^*$  to obtain  $\Sigma_{\text{Lap}}$ .

## 7. Detailed Derivation of Gradient and Hessian

For completeness, we include the full derivation of the gradient and Hessian of  $E(p)$ .

Recall:

$$E(p) = M(p) + P(p), \quad M(p) = \frac{\delta^2}{V}, \quad P(p) = (p - \mu) (N_{\text{ch}} \Sigma_p^{-1}) (p - \mu)^\top,$$

with

$$\delta = y - N_{\text{ch}}(p \cdot \gamma), \quad V = \epsilon^2 + N_{\text{ch}}(p \cdot \sigma^2).$$

Here  $p$  is a row vector,  $\gamma$  and  $\sigma^2$  are column vectors.

### 7.1 Prior Gradient and Hessian

Define the precision matrix  $\Lambda_p = N_{\text{ch}} \Sigma_p^{-1}$ . Then:

$$P(p) = (p - \mu) \Lambda_p (p - \mu)^\top.$$

Using the standard formula for the gradient of a quadratic form  $f(p) = (p - \mu) A (p - \mu)^\top$ , with symmetric  $A$ , we have:

$$\nabla f(p) = 2(p - \mu) A,$$

and

$$\nabla^2 f(p) = 2A.$$

Thus:

$$\begin{aligned} \nabla P(p) &= 2(p - \mu) \Lambda_p = 2N_{\text{ch}}(p - \mu) \Sigma_p^{-1}, \\ \nabla^2 P(p) &= 2\Lambda_p = 2N_{\text{ch}} \Sigma_p^{-1}. \end{aligned}$$

### 7.2 Likelihood Gradient

We have:

$$M(p) = \frac{\delta^2}{V}, \quad \delta = y - N_{\text{ch}}(p \cdot \gamma), \quad V = \epsilon^2 + N_{\text{ch}}(p \cdot \sigma^2).$$

First compute the gradients of  $\delta$  and  $V$ :

$$\nabla \delta(p) = -N_{\text{ch}} \gamma^\top, \quad \nabla V(p) = N_{\text{ch}}(\sigma^2)^\top,$$

both row vectors.

Now apply the quotient rule to  $M(p) = \delta^2/V$ :

$$\nabla M(p) = \frac{2\delta}{V} \nabla \delta - \frac{\delta^2}{V^2} \nabla V.$$

Substituting:

$$\nabla M(p) = \frac{2\delta}{V} (-N_{\text{ch}} \gamma^\top) - \frac{\delta^2}{V^2} N_{\text{ch}} (\sigma^2)^\top = -N_{\text{ch}} \left[ \frac{2\delta}{V} \gamma^\top + \frac{\delta^2}{V^2} (\sigma^2)^\top \right].$$

### 7.3 Likelihood Hessian

Write:

$$M(p) = \delta^2 V^{-1}.$$

We already have:

$$\nabla M(p) = a(p) \nabla \delta(p) - b(p) \nabla V(p),$$

with:

$$a(p) = \frac{2\delta}{V}, \quad b(p) = \frac{\delta^2}{V^2}.$$

Because  $\delta$  and  $V$  are affine in  $p$ , their Hessians vanish:  $\nabla^2 \delta = 0$ ,  $\nabla^2 V = 0$ . Thus:

$$\nabla^2 M(p) = (\nabla a) \nabla \delta - (\nabla b) \nabla V.$$

It remains to compute  $\nabla a$  and  $\nabla b$ .

**Gradient of  $a(p)$ .**

$$a(p) = \frac{2\delta}{V}.$$

Using the quotient rule:

$$\nabla a = \frac{2}{V} \nabla \delta - \frac{2\delta}{V^2} \nabla V.$$

Substitute:

$$\nabla a = \frac{2}{V} (-N_{\text{ch}} \gamma^\top) - \frac{2\delta}{V^2} N_{\text{ch}} (\sigma^2)^\top = -\frac{2N_{\text{ch}}}{V} \gamma^\top - \frac{2N_{\text{ch}}\delta}{V^2} (\sigma^2)^\top.$$

**Gradient of  $b(p)$ .**

$$b(p) = \frac{\delta^2}{V^2}.$$

Differentiating:

$$\nabla b = 2 \frac{\delta}{V^2} \nabla \delta - 2 \frac{\delta^2}{V^3} \nabla V.$$

Substitute:

$$\nabla b = 2 \frac{\delta}{V^2} (-N_{\text{ch}} \gamma^\top) - 2 \frac{\delta^2}{V^3} N_{\text{ch}} (\sigma^2)^\top = -\frac{2N_{\text{ch}}\delta}{V^2} \gamma^\top - \frac{2N_{\text{ch}}\delta^2}{V^3} (\sigma^2)^\top.$$

**Assembling the Hessian.** Recall:

$$\nabla^2 M(p) = (\nabla a) \nabla \delta - (\nabla b) \nabla V.$$

Using:

$$\nabla \delta = -N_{\text{ch}} \gamma^\top, \quad \nabla V = N_{\text{ch}} (\sigma^2)^\top,$$

we obtain:

$$\nabla^2 M(p) = (\nabla a) (-N_{\text{ch}} \gamma^\top) - (\nabla b) N_{\text{ch}} (\sigma^2)^\top.$$

Substituting the expressions for  $\nabla a$  and  $\nabla b$  and collecting terms, we arrive at:

$$\nabla^2 M(p) = 2N_{\text{ch}}^2 \left[ \frac{1}{V} \gamma \gamma^\top + \frac{\delta}{V^2} (\gamma (\sigma^2)^\top + \sigma^2 \gamma^\top) + \frac{\delta^2}{V^3} \sigma^2 (\sigma^2)^\top \right].$$

## 7.4 Full Gradient and Hessian

Combining prior and likelihood:

$$\begin{aligned} \mathbf{g}(p) &= \nabla E(p) = \nabla M(p) + \nabla P(p) \\ &= 2N_{\text{ch}}(p - \mu) \Sigma_p^{-1} - N_{\text{ch}} \left[ \frac{2\delta}{V} \gamma^\top + \frac{\delta^2}{V^2} (\sigma^2)^\top \right], \end{aligned}$$

and:

$$\begin{aligned} \mathbf{H}(p) &= \nabla^2 E(p) = \nabla^2 M(p) + \nabla^2 P(p) \\ &= 2N_{\text{ch}} \Sigma_p^{-1} + 2N_{\text{ch}}^2 \left[ \frac{1}{V} \gamma \gamma^\top + \frac{\delta}{V^2} (\gamma (\sigma^2)^\top + \sigma^2 \gamma^\top) + \frac{\delta^2}{V^3} \sigma^2 (\sigma^2)^\top \right]. \end{aligned}$$

## 7.5 Rank-1 Factorisation of the Hessian

Define:

$$v = \gamma + \frac{\delta}{V}\sigma^2.$$

Compute:

$$vv^\top = \gamma\gamma^\top + \frac{\delta}{V}(\gamma(\sigma^2)^\top + \sigma^2\gamma^\top) + \frac{\delta^2}{V^2}\sigma^2(\sigma^2)^\top.$$

Then:

$$\frac{N_{\text{ch}}}{V}vv^\top = \frac{N_{\text{ch}}}{V}\gamma\gamma^\top + \frac{N_{\text{ch}}\delta}{V^2}(\gamma(\sigma^2)^\top + \sigma^2\gamma^\top) + \frac{N_{\text{ch}}\delta^2}{V^3}\sigma^2(\sigma^2)^\top,$$

which matches exactly the bracketed term in the expression for  $\nabla^2 M(p)$ , scaled by  $2N_{\text{ch}}^2$ .

Thus:

$$\nabla^2 M(p) = 2N_{\text{ch}}^2 \frac{1}{V}vv^\top,$$

and so the full Hessian is:

$$\mathbf{H}(p) = 2N_{\text{ch}}\Sigma_p^{-1} + 2N_{\text{ch}}^2 \frac{1}{V}vv^\top = 2N_{\text{ch}} \left[ \Sigma_p^{-1} + \frac{N_{\text{ch}}}{V}vv^\top \right].$$

Introducing

$$u = \sqrt{\frac{N_{\text{ch}}}{V}} v,$$

we recover:

$$\mathbf{H}(p) = 2N_{\text{ch}}(\Sigma_p^{-1} + uu^\top),$$

which is the starting point for the Sherman–Morrison inversion in Section 4.

This completes the detailed derivation with consistent vector orientations, explicit dependence of  $\delta$ ,  $V$  and  $v$  on  $p$ , and with all explicit uses of  $\Sigma_p^{-1}$  eliminated from the implementable formulas for  $p_{\text{post}}$  and  $\Sigma_{\text{post}}$ .

## 8. Exact MAP Energy with $\log V$ and Rank-2 Hessian

In the previous sections we defined the energy as

$$E_{\text{quasi}}(p) = \frac{\delta(p)^2}{V(p)} + (p - \mu)(N_{\text{ch}}\Sigma_p^{-1})(p - \mu)^\top,$$

which corresponds to a *quasi-likelihood* that uses  $V(p)$  only as a weight for the squared residual. This choice yields a rank-1 Hessian update and a simple closed form for  $\Sigma_{\text{post}}$ .

If we take seriously the generative model

$$y \mid p \sim \mathcal{N}(N_{\text{ch}}(p \cdot \gamma), V(p)),$$

then the *exact* negative log-likelihood (up to an additive constant) is

$$E_{\text{like}}(p) = \log V(p) + \frac{\delta(p)^2}{V(p)}.$$

In this section we incorporate the  $\log V(p)$  term and work with the *exact* negative log-posterior

$$E_{\text{exact}}(p) = \underbrace{\log V(p) + \frac{\delta(p)^2}{V(p)}}_{\text{data}} + \underbrace{(p - \mu)(N_{\text{ch}}\Sigma_p^{-1})(p - \mu)^\top}_{\text{prior}} + \text{const.}$$

As before:

$$\delta(p) = y - N_{\text{ch}}(p \cdot \gamma), \quad V(p) = \epsilon^2 + N_{\text{ch}}(p \cdot \sigma^2),$$

and

$$v(p) = \gamma + \frac{\delta(p)}{V(p)} \sigma^2.$$

The prior log-determinant term (pseudo-determinant of the singular  $\Sigma_p$ ) is a constant in  $p$  and therefore *does not* affect the MAP; we ignore it here.

## 8.1 Exact Gradient

We decompose

$$E_{\text{exact}}(p) = L(p) + M(p) + P(p),$$

with

$$L(p) = \log V(p), \quad M(p) = \frac{\delta(p)^2}{V(p)}, \quad P(p) = (p - \mu)(N_{\text{ch}}\Sigma_p^{-1})(p - \mu)^\top.$$

The gradients of  $M$  and  $P$  were already computed in Section 7:

$$\nabla M(p) = -N_{\text{ch}} \left[ \frac{2\delta(p)}{V(p)} \gamma^\top + \frac{\delta(p)^2}{V(p)^2} (\sigma^2)^\top \right],$$

$$\nabla P(p) = 2N_{\text{ch}}(p - \mu)\Sigma_p^{-1}.$$

For the new term  $L(p) = \log V(p)$  we have

$$\nabla L(p) = \frac{1}{V(p)} \nabla V(p) = \frac{N_{\text{ch}}}{V(p)} (\sigma^2)^\top,$$

since  $\nabla V(p) = N_{\text{ch}}(\sigma^2)^\top$ .

Thus the *exact* gradient becomes

$$\mathbf{g}_{\text{exact}}(p) = \nabla E_{\text{exact}}(p) = 2N_{\text{ch}}(p - \mu)\Sigma_p^{-1} - N_{\text{ch}} \left[ \frac{2\delta(p)}{V(p)} \gamma^\top + \frac{\delta(p)^2}{V(p)^2} (\sigma^2)^\top - \frac{1}{V(p)} (\sigma^2)^\top \right].$$

Equivalently, grouping the  $(\sigma^2)^\top$  terms:

$$\boxed{\mathbf{g}_{\text{exact}}(p) = 2N_{\text{ch}}(p - \mu)\Sigma_p^{-1} - N_{\text{ch}} \left[ \frac{2\delta(p)}{V(p)} \gamma^\top + \left( \frac{\delta(p)^2}{V(p)^2} - \frac{1}{V(p)} \right) (\sigma^2)^\top \right].}$$

This is what must be used in a true Newton iteration targeting the exact MAP.

## 8.2 Exact Hessian and Rank-2 Structure

We now add the Hessian of  $L(p)$  to the Hessian derived in Section 7 for  $M(p) + P(p)$ .

From Section 7:

$$\nabla^2 P(p) = 2N_{\text{ch}}\Sigma_p^{-1},$$

$$\nabla^2 M(p) = 2N_{\text{ch}}^2 \left[ \frac{1}{V(p)} \gamma\gamma^\top + \frac{\delta(p)}{V(p)^2} (\gamma(\sigma^2)^\top + \sigma^2\gamma^\top) + \frac{\delta(p)^2}{V(p)^3} \sigma^2\sigma^{2\top} \right].$$

For  $L(p) = \log V(p)$ , using  $\nabla V(p) = N_{\text{ch}}(\sigma^2)^\top$  and  $\nabla^2 V(p) = 0$ :

$$\nabla^2 L(p) = -\frac{1}{V(p)^2} (\nabla V(p))^\top \nabla V(p) = -\frac{N_{\text{ch}}^2}{V(p)^2} \sigma^2\sigma^{2\top}.$$

Therefore:

$$\nabla^2 (M(p) + L(p)) = 2N_{\text{ch}}^2 \left[ \frac{1}{V(p)} \gamma\gamma^\top + \frac{\delta(p)}{V(p)^2} (\gamma(\sigma^2)^\top + \sigma^2\gamma^\top) + \left( \frac{\delta(p)^2}{V(p)^3} - \frac{1}{2V(p)^2} \right) \sigma^2\sigma^{2\top} \right].$$

Adding the prior Hessian,

$$\nabla^2 P(p) = 2N_{\text{ch}}\Sigma_p^{-1},$$



we obtain the full exact Hessian:

$$\mathbf{H}_{\text{exact}}(p) = 2N_{\text{ch}}\Sigma_p^{-1} + 2N_{\text{ch}}^2 \left[ \frac{1}{V(p)} \gamma \gamma^\top + \frac{\delta(p)}{V(p)^2} (\gamma(\sigma^2)^\top + \sigma^2 \gamma^\top) + \left( \frac{\delta(p)^2}{V(p)^3} - \frac{1}{2V(p)^2} \right) \sigma^2 \sigma^{2\top} \right].$$

It is convenient to rewrite this as a *rank-2* update of the prior precision. As before, define

$$v(p) = \gamma + \frac{\delta(p)}{V(p)} \sigma^2,$$

and let

$$u_1(p) = v(p), \quad u_2(p) = \sigma^2.$$

We will write the Hessian in the form

$$\mathbf{H}_{\text{exact}}(p) = 2N_{\text{ch}} [\Sigma_p^{-1} + U(p)C(p)U(p)^\top],$$

with

$$U(p) = [u_1(p), u_2(p)] \in \mathbb{R}^{d \times 2},$$

and  $C(p)$  a  $2 \times 2$  diagonal matrix.

From the rank-1 case we know that

$$\frac{N_{\text{ch}}}{V(p)} v(p)v(p)^\top = \frac{N_{\text{ch}}}{V(p)} u_1(p)u_1(p)^\top$$

generates the  $M$ -part of the Hessian without  $\log V$ . The extra term from  $L(p)$  is

$$-\frac{N_{\text{ch}}^2}{V(p)^2} \sigma^2 \sigma^{2\top} = 2N_{\text{ch}} \left( -\frac{N_{\text{ch}}}{2V(p)^2} \right) u_2(p)u_2(p)^\top.$$

Thus we can take

$$C(p) = \begin{pmatrix} \alpha(p) & 0 \\ 0 & \beta(p) \end{pmatrix}, \quad \alpha(p) = \frac{N_{\text{ch}}}{V(p)}, \quad \beta(p) = -\frac{N_{\text{ch}}}{2V(p)^2},$$

so that

$$U(p)C(p)U(p)^\top = \alpha(p)u_1(p)u_1(p)^\top + \beta(p)u_2(p)u_2(p)^\top.$$

We have therefore

$$\boxed{\mathbf{H}_{\text{exact}}(p) = 2N_{\text{ch}} [\Sigma_p^{-1} + U(p)C(p)U(p)^\top]},$$

with a *rank-2* update governed by  $v(p)$  and  $\sigma^2$ .

### 8.3 Woodbury Inversion and Exact Laplace Covariance

The Woodbury identity for a rank- $k$  update says that, for invertible  $A$ ,

$$(A + UCU^\top)^{-1} = A^{-1} - A^{-1}U(C^{-1} + U^\top A^{-1}U)^{-1}U^\top A^{-1},$$

where  $U$  is  $d \times k$  and  $C$  is  $k \times k$ .

We apply this in the intrinsic  $(d-1)$ -dimensional subspace with

$$A = \Sigma_p^{-1}, \quad A^{-1} = \Sigma_p, \quad U = U(p_0), \quad C = C(p_0),$$

for an expansion point  $p_0$ . Then

$$(\Sigma_p^{-1} + UCU^\top)^{-1} = \Sigma_p - \Sigma_p U K U^\top \Sigma_p,$$

where

$$K = (C^{-1} + U^\top \Sigma_p U)^{-1} \in \mathbb{R}^{2 \times 2}.$$

Since

$$\mathbf{H}_{\text{exact}}(p_0) = 2N_{\text{ch}}(\Sigma_p^{-1} + UCU^\top),$$

we get

$$\mathbf{H}_{\text{exact}}(p_0)^{-1} = \frac{1}{2N_{\text{ch}}} \left[ \Sigma_p - \Sigma_p U K U^\top \Sigma_p \right].$$

The *exact* Laplace covariance at  $p_0$  is

$$\Sigma_{\text{post}}^{\text{exact}}(p_0) = 2\mathbf{H}_{\text{exact}}(p_0)^{-1} = \frac{1}{N_{\text{ch}}} \left[ \Sigma_p - \Sigma_p U K U^\top \Sigma_p \right].$$

Explicitly, at  $p_0$ :

$$U = [v(p_0), \sigma^2], \quad C = \begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix},$$

with

$$\alpha = \frac{N_{\text{ch}}}{V(p_0)}, \quad \beta = -\frac{N_{\text{ch}}}{2V(p_0)^2}.$$

The  $2 \times 2$  matrix

$$M = C^{-1} + U^\top \Sigma_p U$$

is

$$M = \begin{pmatrix} \alpha^{-1} + v^\top \Sigma_p v & v^\top \Sigma_p \sigma^2 \\ \sigma^{2\top} \Sigma_p v & \beta^{-1} + \sigma^{2\top} \Sigma_p \sigma^2 \end{pmatrix} = \begin{pmatrix} \frac{V}{N_{\text{ch}}} + s & b \\ b & -\frac{2V(p_0)^2}{N_{\text{ch}}} + c \end{pmatrix},$$

where

$$s = v^\top \Sigma_p v, \quad b = v^\top \Sigma_p \sigma^2, \quad c = \sigma^2 \Sigma_p \sigma^2.$$

Then

$$K = M^{-1}$$

is the inverse of a *2-by-2* matrix, which can always be computed analytically or numerically with negligible cost relative to the channel-ensemble computations.

Thus the exact MAP covariance is

$$\Sigma_{\text{post}}^{\text{exact}}(p_0) = \frac{1}{N_{\text{ch}}} \left[ \Sigma_p - \Sigma_p U(p_0) K(p_0) U(p_0)^\top \Sigma_p \right],$$

with  $K(p_0) = (C(p_0)^{-1} + U(p_0)^\top \Sigma_p U(p_0))^{-1}$ .

**Remark (singular prior).** Again,  $\Sigma_p^{-1}$  appears only formally in the Woodbury algebra. The implementable expression for  $\Sigma_{\text{post}}^{\text{exact}}(p_0)$  contains only  $\Sigma_p$ ,  $U(p_0)$  and the small  $2 \times 2$  inverse  $K(p_0)$ .

## 8.4 Exact Mean Update and Elimination of $\Sigma_p^{-1}$

The exact Laplace mean at  $p_0$  is

$$p_{\text{post}}^{\text{exact}} = p_0 - \mathbf{g}_{\text{exact}}(p_0) \mathbf{H}_{\text{exact}}(p_0)^{-1} = p_0 - \frac{1}{2} \mathbf{g}_{\text{exact}}(p_0) \Sigma_{\text{post}}^{\text{exact}}(p_0).$$

Write

$$\Delta p = p_0 - \mu,$$

and decompose the gradient as

$$\mathbf{g}_{\text{exact}}(p_0) = 2N_{\text{ch}} \Delta p \Sigma_p^{-1} - N_{\text{ch}} q^\top,$$

where

$$q^\top = \frac{2\delta}{V} \gamma^\top + \left( \frac{\delta^2}{V^2} - \frac{1}{V} \right) (\sigma^2)^\top,$$

with  $\delta = \delta(p_0)$  and  $V = V(p_0)$ .

Then

$$p_{\text{post}}^{\text{exact}} = p_0 - N_{\text{ch}} \Delta p \Sigma_p^{-1} \Sigma_{\text{post}}^{\text{exact}}(p_0) + \frac{N_{\text{ch}}}{2} q^\top \Sigma_{\text{post}}^{\text{exact}}(p_0).$$

Using the exact covariance expression

$$\Sigma_{\text{post}}^{\text{exact}}(p_0) = \frac{1}{N_{\text{ch}}} \left[ \Sigma_p - \Sigma_p U K U^\top \Sigma_p \right],$$

we compute

$$\begin{aligned} \Sigma_p^{-1} \Sigma_{\text{post}}^{\text{exact}}(p_0) &= \Sigma_p^{-1} \left[ \frac{1}{N_{\text{ch}}} (\Sigma_p - \Sigma_p U K U^\top \Sigma_p) \right] \\ &= \frac{1}{N_{\text{ch}}} (I - U K U^\top \Sigma_p). \end{aligned}$$

Thus

$$N_{\text{ch}} \Delta p \Sigma_p^{-1} \Sigma_{\text{post}}^{\text{exact}}(p_0) = \Delta p - \Delta p U K U^\top \Sigma_p.$$

Substituting back:

$$\begin{aligned} p_{\text{post}}^{\text{exact}} &= p_0 - \left[ \Delta p - \Delta p U K U^\top \Sigma_p \right] + \frac{N_{\text{ch}}}{2} q^\top \Sigma_{\text{post}}^{\text{exact}}(p_0) \\ &= (p_0 - \Delta p) + \Delta p U K U^\top \Sigma_p + \frac{N_{\text{ch}}}{2} q^\top \Sigma_{\text{post}}^{\text{exact}}(p_0). \end{aligned}$$

Since  $p_0 - \Delta p = \mu$ , we obtain the exact mean update in a form with no explicit  $\Sigma_p^{-1}$ :

$$\boxed{p_{\text{post}}^{\text{exact}} = \mu + \Delta p U(p_0) K(p_0) U(p_0)^\top \Sigma_p + \frac{N_{\text{ch}}}{2} q^\top \Sigma_{\text{post}}^{\text{exact}}(p_0),}$$

with

$$\Delta p = p_0 - \mu, \quad q^\top = \frac{2\delta}{V} \gamma^\top + \left( \frac{\delta^2}{V^2} - \frac{1}{V} \right) (\sigma^2)^\top,$$

and  $\Sigma_{\text{post}}^{\text{exact}}(p_0)$  given above.

## 8.5 Summary: Rank-1 vs Rank-2 Schemes

We now have two related Laplace schemes:

- **Quasi-Laplace (rank-1):**

- Energy:  $E_{\text{quasi}}(p) = \delta(p)^2/V(p) + P(p)$ .
- Hessian: rank-1 update, closed form  $\Sigma_{\text{post}}(p_0) = \frac{1}{N_{\text{ch}}} \Sigma_p - \frac{1}{V(p_0) + N_{\text{ch}} s(p_0)} \Sigma_p v(p_0) v(p_0)^\top$
- Mean update: Eq. (2) in Section 5, no explicit  $\Sigma_p^{-1}$ .

- **Exact MAP + Laplace (rank-2):**

- Energy:  $E_{\text{exact}}(p) = \log V(p) + \delta(p)^2/V(p) + P(p)$ .
- Hessian: rank-2 update,  $\mathbf{H}_{\text{exact}}(p) = 2N_{\text{ch}}[\Sigma_p^{-1} + U(p)C(p)U(p)^\top]$ .
- Covariance:  $\Sigma_{\text{post}}^{\text{exact}}(p_0) = \frac{1}{N_{\text{ch}}}[\Sigma_p - \Sigma_p U(p_0)K(p_0)U(p_0)^\top \Sigma_p]$ ,  
with a  $2 \times 2$  matrix  $K(p_0)$ .
- Mean update: the exact expression above, again without explicit  $\Sigma_p^{-1}$ .

From an implementation perspective, the heavy lifting in MacroIR/MacroDR remains the computation of the channel-ensemble statistics that define  $\gamma$ ,  $\sigma^2$ , and thus  $V(p)$  and  $v(p)$ . Going from a rank-1 to a rank-2 Hessian only requires a  $2 \times 2$  matrix inversion per interval, which is negligible compared to the cost of the boundary-state and tilde-operator computations.

## 8. Exact MAP from the Gaussian Likelihood (with $\frac{1}{2}$ factors)

Up to now we have worked with an “energy”

$$E(p) = M(p) + P(p)$$

(and in Section 8 with  $E_{\text{exact}}(p) = L(p) + M(p) + P(p)$ ) without explicit  $\frac{1}{2}$  factors. In this section we start from the *actual* Gaussian likelihood and prior, write the *true* negative log-posterior, and then explain how it relates to the energies used in the rest of the note.

### 8.1 Gaussian likelihood and prior in standard form

Given a macroscopic state  $p$ , the scalar interval-averaged current is modelled as

$$y \mid p \sim \mathcal{N}(\mu_y(p), V(p)), \quad \mu_y(p) = N_{\text{ch}}(p \cdot \gamma),$$

with

$$V(p) = \epsilon^2 + N_{\text{ch}}(p \cdot \sigma^2).$$

The Gaussian likelihood is

$$p(y \mid p) = \frac{1}{\sqrt{2\pi V(p)}} \exp\left(-\frac{1}{2} \frac{(y - \mu_y(p))^2}{V(p)}\right).$$

Define

$$\delta(p) = y - N_{\text{ch}}(p \cdot \gamma),$$

so that

$$p(y | p) = \frac{1}{\sqrt{2\pi V(p)}} \exp\left(-\frac{1}{2} \frac{\delta(p)^2}{V(p)}\right).$$

The log-likelihood is therefore

$$\log p(y | p) = -\frac{1}{2} \log(2\pi) - \frac{1}{2} \log V(p) - \frac{1}{2} \frac{\delta(p)^2}{V(p)}.$$

Ignoring the constant  $-\frac{1}{2} \log(2\pi)$ , the *negative* log-likelihood is

$$F_{\text{like}}(p) = \frac{1}{2} \log V(p) + \frac{1}{2} \frac{\delta(p)^2}{V(p)} \quad (+ \text{ const}).$$

For the prior we assume

$$p \sim \mathcal{N}(\mu, \Sigma_p)$$

on the simplex, with precision

$$\Lambda_p = N_{\text{ch}} \Sigma_p^{-1}.$$

The prior density is

$$p(p) \propto \exp\left(-\frac{1}{2} (p - \mu) \Lambda_p (p - \mu)^\top\right),$$

so the negative log-prior (up to a constant) is

$$F_{\text{prior}}(p) = \frac{1}{2} (p - \mu) \Lambda_p (p - \mu)^\top = \frac{1}{2} (p - \mu) (N_{\text{ch}} \Sigma_p^{-1}) (p - \mu)^\top.$$

## 8.2 Exact negative log-posterior and scaling to “energy”

The (unnormalised) posterior is

$$p(p | y) \propto p(y | p) p(p),$$

so the *exact* negative log-posterior is

$$F_{\text{exact}}(p) = F_{\text{like}}(p) + F_{\text{prior}}(p) \quad (+ \text{ const}),$$

that is

$$F_{\text{exact}}(p) = \frac{1}{2} \log V(p) + \frac{1}{2} \frac{\delta(p)^2}{V(p)} + \frac{1}{2} (p - \mu) (N_{\text{ch}} \Sigma_p^{-1}) (p - \mu)^\top \quad (+ \text{const}).$$

This is what one should minimise to obtain the true MAP:

$$p^\star = \arg \min_p F_{\text{exact}}(p).$$

For algebraic convenience in the rest of the note we work with an *energy* that is simply twice the negative log-posterior:

$$E_{\text{exact}}(p) := 2F_{\text{exact}}(p).$$

Up to an additive constant,

$$E_{\text{exact}}(p) = \underbrace{\log V(p) + \frac{\delta(p)^2}{V(p)}}_{L(p)+M(p)} + \underbrace{(p - \mu) (N_{\text{ch}} \Sigma_p^{-1}) (p - \mu)^\top}_{P(p)}.$$

This is exactly the decomposition used in Section 8:

$$E_{\text{exact}}(p) = L(p) + M(p) + P(p).$$

*Important:* multiplying  $F_{\text{exact}}$  by a positive constant does not change the MAP. Moreover, since

$$E_{\text{exact}}(p) = 2F_{\text{exact}}(p),$$

their Hessians satisfy

$$\nabla^2 E_{\text{exact}}(p) = 2 \nabla^2 F_{\text{exact}}(p),$$

and the Laplace covariance of the posterior,

$$\Sigma_{\text{Lap}} \approx [\nabla^2 F_{\text{exact}}(p^\star)]^{-1},$$

can be computed as

$$\Sigma_{\text{Lap}} = 2[\nabla^2 E_{\text{exact}}(p^\star)]^{-1}.$$

This is exactly the convention used earlier in the note, where we wrote

$$\Sigma_{\text{post}} = 2 \mathbf{H}^{-1}$$

with  $\mathbf{H} = \nabla^2 E$ .

Thus:

- all gradient and Hessian formulas derived for  $E_{\text{exact}}$  (including the rank-2 Woodbury structure in Section 8) are correct and correspond to  $2\times$  the exact negative log-posterior;
- the MAP is obtained by minimising  $F_{\text{exact}}$  or equivalently  $E_{\text{exact}}$ ;
- the Laplace covariance is always  $\Sigma_{\text{Lap}} = 2\mathbf{H}_{\text{exact}}^{-1}$  when  $\mathbf{H}_{\text{exact}} = \nabla^2 E_{\text{exact}}$ .

### 8.3 Exact vs quasi energy

For comparison:

- The *exact* data term from the Gaussian likelihood is

$$F_{\text{like}}(p) = \frac{1}{2} \log V(p) + \frac{1}{2} \frac{\delta(p)^2}{V(p)} \quad (+ \text{const}),$$

and the corresponding energy contribution in this note is

$$L(p) + M(p) = \log V(p) + \frac{\delta(p)^2}{V(p)} = 2F_{\text{like}}(p) \quad (+ \text{const}).$$

- The earlier “quasi” scheme drops the  $\log V(p)$  term and keeps only  $\delta(p)^2/V(p)$  (again up to a factor 2), which yields a rank-1 Hessian and the simpler covariance formula.

In other words:

- if you want the *exact* Gaussian MAP, work with  $F_{\text{exact}}$  defined above; all rank-2 Hessian and Woodbury formulas in Section 8 apply directly via  $E_{\text{exact}} = 2F_{\text{exact}}$  and  $\Sigma_{\text{Lap}} = 2\mathbf{H}_{\text{exact}}^{-1}$ ;
- if you are happy with the quasi-likelihood (no  $\log V$  term), you can use the rank-1 scheme from the earlier sections.