MacroIR Interval Update
Unified Boundary-State and Tilde Operator Specification

0 Scope and conventions

We consider an ensemble of N_{ch} independent Markov channels with K microscopic states. Over an interval $[0, t]$ we observe a scalar interval-averaged macroscopic current $\overline{y}^{\mathrm{obs}}_{0\to t}$. We want the posterior mean and covariance of the macroscopic state at time t, and the predictive mean and variance of the interval current.

Convention. In what follows:

- $(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$ describe the per-channel occupancy statistics at the start of the interval:
  - $\mu_{0,i} = \mathbb{E}[\text{fraction of channels in state } i]$,
  - $\sum_i \mu_{0,i} = 1$.
- Macroscopic means and variances are expressed per ion channel; total currents and variances scale with N_{ch}.

You can convert to raw counts as $\boldsymbol{n}_0 = N_{\mathrm{ch}}\boldsymbol{\mu}_0$ if needed; all formulas simply scale accordingly.

1 Indices, shapes, and operators

- K: number of microscopic states.
- Indices:
  - i_0, j_0: start (time 0) states.
  - i_t, j_t: end (time t) states.
  - a, b: generic state indices at time t.
- State vectors are columns:

$$\boldsymbol{\mu}_0 \in \mathbb{R}^K, \quad \boldsymbol{\mu}^{\mathrm{prior}}(t) \in \mathbb{R}^K, \text{ etc.}$$

- State-property vectors are columns:

$$\overline{\boldsymbol{\gamma}}_0 \in \mathbb{R}^K, \quad \boldsymbol{\sigma}^2_{\overline{\gamma}_0} \in \mathbb{R}^K, \text{ etc.}$$

- State covariance matrices are indexed by two states at the same time:

$$\boldsymbol{\Sigma}_0,\ \boldsymbol{\Sigma}^{\mathrm{prop}}_t \in \mathbb{R}^{K\times K} \quad \text{(symmetric)}.$$

- State transition and boundary-property matrices are indexed by the state at start time 0, i_0, and at end time t, i_t:
  - $\mathbf{P}(t) \in \mathbb{R}^{K\times K}$ with entries $P_{i_0\to i_t}(t)$ (asymmetric; $\sum_{i_t} P_{i_0\to i_t}(t) = 1$; row sums are 1).
  - Mean and variance-of-mean conductance matrices $\overline{\mathbf{\Gamma}}, \overline{\mathbf{V}} \in \mathbb{R}^{K\times K}$ indexed by $(i_0 \to i_t)$.
- Elementwise (Hadamard) product: $A \circ B$.
- $\mathrm{diag}(x)$: diagonal matrix from vector x.
- $\mathrm{diag}(A)$: vector of diagonal entries of matrix A.
- $\mathbf{1}$: all-ones column vector in $\mathbb{R}^K$.

2 Inputs and precomputed microscopic objects

For each interval $[0, t]$ we need:

2.1 Macroscopic prior

- $\boldsymbol{\mu}_0$,
- $\mathbf{\Sigma}_0$ (covariance at time 0).

2.2 Markov dynamics

- Generator $\mathbf{Q}$ (offline).
- Transition matrix

$$\mathbf{P}(t) = e^{\mathbf{Q}t}, \qquad P_{i_0\to i_t}(t) = [\mathbf{P}(t)]_{i_0 i_t}.$$

2.3 Boundary-conditioned current statistics

- Mean interval current (per channel, conditioned on boundary states):

$$\overline{\Gamma}_{i_0\to i_t} = \mathbb{E}\left[\frac{1}{t}\int_0^t y(\tau)\,\mathrm{d}\tau \,\middle|\, i_0, i_t\right].$$

- Variance contribution (intrinsic interval noise, per channel, conditioned on boundary states):

$$\overline{V}_{i_0\to i_t} = \mathrm{Var}\left(\frac{1}{t}\int_0^t y(\tau)\,\mathrm{d}\tau \,\middle|\, i_0, i_t\right).$$

2.4 Measurement setup

- Number of channels N_{ch}.
- Instrument/binning noise:

$$\epsilon_{0\to t}^2 = \frac{\epsilon^2}{t} + \nu^2.$$

- Observation $\overline{y}_{0\to t}^{\mathrm{obs}}$.

3 Boundary-state representation: the core insight

3.1 The boundary-state trick

Introduce *boundary states* (i_0, i_t) representing start–end pairs. For each boundary pair, precompute:

- Mean interval-averaged current: $\overline{\Gamma}_{i_0 \to i_t}$.
- Intrinsic variance contribution: $\overline{V}_{i_0 \to i_t}$.

These are arranged in $K \times K$ matrices

$$\overline{\mathbf{\Gamma}}, \quad \overline{\mathbf{V}},$$

indexed by (i_0, i_t).

3.2 Boundary-state random variables

For the ensemble, define the boundary count

$$N_{i_0 \to i_t} = \text{number of channels that start in } i_0 \text{ and end in } i_t.$$

The *boundary-state mean* is

$$\mu^{\text{prior}}_{0 \to t, (i_0 \to i_t)} = \mathbb{E}[N_{i_0 \to i_t}] = (\boldsymbol{\mu}_0)_{i_0} \, P_{i_0 \to i_t}(t).$$

A convenient decomposition of the (per-channel-normalised) *boundary-state covariance* is

$$\begin{aligned} \Sigma^{\text{prior}}_{0 \to t, (i_0 \to i_t)(j_0 \to j_t)} &= P_{i_0 \to i_t}(t) \big[(\mathbf{\Sigma}_0)_{i_0 j_0} - \delta_{i_0 j_0} (\boldsymbol{\mu}_0)_{i_0} \big] P_{j_0 \to j_t}(t) \\ &\quad + \delta_{i_0 j_0} \delta_{i_t j_t} (\boldsymbol{\mu}_0)_{i_0} P_{i_0 \to i_t}(t). \end{aligned}$$

This separates:

- the propagated *initial covariance* $\mathbf{\Sigma}_0$, and
- the *multinomial splitting noise* within each start state.

3.3 Boundary-conditioned expectations

Define the start-indexed conditional mean of the interval current:

$$(\overline{\gamma}_0)_{i_0} = \sum_{i_t} P_{i_0 \to i_t}(t) \, \overline{\Gamma}_{i_0 \to i_t}.$$

Similarly, the intrinsic variance conditioned on i_0:

$$(\sigma^2_{\overline{\gamma}_0})_{i_0} = \sum_{i_t} P_{i_0 \to i_t}(t) \, \overline{V}_{i_0 \to i_t}.$$

4 Boundary-lifted current statistics

Define

$$\mathbf{G} = \overline{\mathbf{\Gamma}} \circ \mathbf{P}(t), \qquad G_{i_0 i_t} = \overline{\Gamma}_{i_0 \to i_t} P_{i_0 \to i_t}(t).$$

4.1 Start-conditioned mean interval current

Component-wise:

$$(\overline{\gamma}_0)_{i_0} = \sum_{i_t} G_{i_0 i_t}.$$

Matrix form:

$$\overline{\boldsymbol{\gamma}}_0 = \mathbf{G}\mathbf{1}.$$

4.2 Start-conditioned intrinsic variance

Define

$$\mathbf{V} = \overline{\mathbf{V}} \circ \mathbf{P}(t),$$

then

$$(\sigma^2_{\overline{\gamma}_0})_{i_0} = \sum_{i_t} V_{i_0 i_t}.$$

Matrix form:

$$\boldsymbol{\sigma}^2_{\overline{\gamma}_0} = \mathbf{V}\mathbf{1}.$$

5 Predictive mean of the interval current

The predictive mean interval current (per ensemble) is

$$\boxed{\overline{y}^{\text{pred}}_{0\to t} = N_{\text{ch}}\, \boldsymbol{\mu}_0^\top \overline{\boldsymbol{\gamma}}_0}.$$

6 The tilde operator

We now define a unified family of operators that couple prior moments $(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$, the transition matrix $\mathbf{P}(t)$, and boundary matrices such as $\overline{\boldsymbol{\Gamma}}$.

6.1 Tilde over mean state: $\widetilde{\boldsymbol{\mu}_0}$mu-tilde

The propagated mean at time t is

$$\boxed{\widetilde{\boldsymbol{\mu}_0} = \mathbf{P}(t)^\top \boldsymbol{\mu}_0}.$$

6.2 Tilde over state covariance: $\widetilde{\boldsymbol{\Sigma}_0}$Sigma-tilde

The propagated covariance at time t is

$$\boxed{\widetilde{\boldsymbol{\Sigma}_0} = \mathbf{P}(t)^\top \big(\boldsymbol{\Sigma}_0 - \operatorname{diag}(\boldsymbol{\mu}_0)\big)\mathbf{P}(t) + \operatorname{diag}\big(\mathbf{P}(t)^\top \boldsymbol{\mu}_0\big)}.$$

This is the usual "linear propagation plus process noise" decomposition for multinomial splitting.

6.3 Tilde over bilinear product: $\widetilde{u^\top \Sigma w}$uTSigmaw-tilde

Let $\overline{\mathbf{U}}, \overline{\mathbf{W}} \in \mathbb{R}^{K\times K}$ be boundary-property matrices (analogous to $\overline{\mathbf{\Gamma}}$), and define the start-conditioned expectations

$$\overline{\boldsymbol{u}}_0 = (\overline{\mathbf{U}} \circ \mathbf{P}(t))\mathbf{1}, \qquad \overline{\boldsymbol{w}}_0 = (\overline{\mathbf{W}} \circ \mathbf{P}(t))\mathbf{1}.$$

Then the bilinear tilde is

$$\boxed{\widetilde{u^\top \Sigma w} = \overline{\boldsymbol{u}}_0^\top \big(\mathbf{\Sigma}_0 - \mathrm{diag}(\boldsymbol{\mu}_0)\big)\overline{\boldsymbol{w}}_0 + \boldsymbol{\mu}_0^\top \big[(\overline{\mathbf{U}} \circ \overline{\mathbf{W}} \circ \mathbf{P}(t))\mathbf{1}\big]}.$$

Interpretation:

- The first term is the action of the propagated initial covariance on the start-conditioned means.
- The second term is the additional variance from within-state multinomial splitting, with a *single* factor of $P_{i_0\to i_t}(t)$ per boundary pair.

Special case: interval current. For the interval current, set $\overline{\mathbf{U}} = \overline{\mathbf{W}} = \overline{\mathbf{\Gamma}}$. Define

$$\mathbf{H} = (\overline{\mathbf{\Gamma}} \circ \overline{\mathbf{\Gamma}}) \circ \mathbf{P}(t), \qquad H_{i_0 i_t} = \overline{\Gamma}^2_{i_0\to i_t} P_{i_0\to i_t}(t).$$

Then

$$\boxed{\widetilde{\gamma^\top \Sigma \gamma} = \overline{\boldsymbol{\gamma}}_0^\top \big(\mathbf{\Sigma}_0 - \mathrm{diag}(\boldsymbol{\mu}_0)\big)\overline{\boldsymbol{\gamma}}_0 + \boldsymbol{\mu}_0^\top \big[\mathbf{H}\mathbf{1}\big]}.$$

Note carefully: the second term involves $\overline{\Gamma}^2_{i_0\to i_t} P_{i_0\to i_t}(t)$, not $\overline{\Gamma}^2_{i_0\to i_t} P^2_{i_0\to i_t}(t)$.

6.4 Vector tilde: $\widetilde{u^\top \Sigma}$uTSigma-tilde

The vector tilde gives the cross-covariance between the state at time t and a boundary-weighted scalar.

For $\overline{\mathbf{U}}$ as above and $\overline{\boldsymbol{u}}_0$ defined as in the previous subsection:

$$\boxed{\widetilde{u^\top \Sigma} = \mathbf{P}(t)^\top \big(\mathbf{\Sigma}_0 - \mathrm{diag}(\boldsymbol{\mu}_0)\big)\overline{\boldsymbol{u}}_0 + (\overline{\mathbf{U}} \circ \mathbf{P}(t))^\top \boldsymbol{\mu}_0}.$$

For the interval current we set $\overline{\mathbf{U}} = \overline{\mathbf{\Gamma}}$, and define

$$\boxed{\mathbf{g} = \widetilde{\gamma^\top \Sigma} = \mathbf{P}(t)^\top \big(\mathbf{\Sigma}_0 - \mathrm{diag}(\boldsymbol{\mu}_0)\big)\overline{\boldsymbol{\gamma}}_0 + \mathbf{G}^\top \boldsymbol{\mu}_0}.$$

7 Predictive variance of the interval current

The predictive variance (per ensemble) decomposes as measurement noise plus contributions from state uncertainty and intrinsic interval noise:

$$\boxed{\sigma^2_{\overline{y}^{\mathrm{pred}}} = \epsilon^2_{0\to t} + N_{\mathrm{ch}}\, \widetilde{\gamma^\top \Sigma \gamma} + N_{\mathrm{ch}}\, \boldsymbol{\mu}_0^\top \boldsymbol{\sigma}^2_{\overline{\gamma}_0}}.$$

8 Propagation to time tt

8.1 Mean

Using the tilde from Section 5.1:

$$\boxed{\boldsymbol{\mu}^{\mathrm{prop}}(t) = \widetilde{\boldsymbol{\mu}_0} = \mathbf{P}(t)^\top \boldsymbol{\mu}_0}.$$

8.2 Covariance

Using the tilde from Section 5.2:

$$\boxed{\boldsymbol{\Sigma}^{\mathrm{prop}}(t) = \widetilde{\boldsymbol{\Sigma}_0} = \mathbf{P}(t)^\top \big(\boldsymbol{\Sigma}_0 - \mathrm{diag}(\boldsymbol{\mu}_0)\big)\mathbf{P}(t) + \mathrm{diag}\big(\boldsymbol{\mu}^{\mathrm{prop}}(t)\big)}.$$

9 Measurement update

Let

$$\delta = \overline{y}^{\mathrm{obs}}_{0\to t} - \overline{y}^{\mathrm{pred}}_{0\to t}.$$

9.1 Mean update

Gaussian conditioning (scalar observation):

$$\boxed{\boldsymbol{\mu}^{\mathrm{post}}(t) = \boldsymbol{\mu}^{\mathrm{prop}}(t) + \frac{\mathbf{g}\,\delta}{\sigma^2_{\overline{y}^{\mathrm{pred}}}}}.$$

9.2 Covariance update

Rank-1 downdate:

$$\boxed{\boldsymbol{\Sigma}^{\mathrm{post}}(t) = \boldsymbol{\Sigma}^{\mathrm{prop}}(t) - \frac{\mathbf{g}\mathbf{g}^\top}{\sigma^2_{\overline{y}^{\mathrm{pred}}}}}.$$

10 Summary of workflow

1. Inputs: $\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0, \mathbf{P}(t), \overline{\boldsymbol{\Gamma}}, \overline{\mathbf{V}}, N_{\mathrm{ch}}, \epsilon^2, \nu^2, \overline{y}^{\mathrm{obs}}_{0\to t}$.
2. Compute:
   - $\mathbf{G} = \overline{\boldsymbol{\Gamma}} \circ \mathbf{P}(t)$.
   - $\overline{\boldsymbol{\gamma}}_0 = \mathbf{G}\mathbf{1}$.
   - $\mathbf{V} = \overline{\mathbf{V}} \circ \mathbf{P}(t)$.
   - $\boldsymbol{\sigma}^2_{\overline{\gamma}_0} = \mathbf{V}\mathbf{1}$.
3. Predictive current:

$$\overline{y}^{\mathrm{pred}}_{0\to t} = N_{\mathrm{ch}}\,\boldsymbol{\mu}_0^\top \overline{\boldsymbol{\gamma}}_0,$$

$$\sigma^2_{\overline{y}^{\mathrm{pred}}} = \epsilon^2_{0\to t} + N_{\mathrm{ch}}\widetilde{\gamma^\top \Sigma \gamma} + N_{\mathrm{ch}}\,\boldsymbol{\mu}_0^\top \boldsymbol{\sigma}^2_{\overline{\gamma}_0}.$$

4. Cross-covariance: $\mathbf{g} = \widetilde{\gamma^\top \Sigma}$ from Section 5.4.

5. Propagate:

   - $\boldsymbol{\mu}^{\text{prop}}(t) = \mathbf{P}(t)^\top \boldsymbol{\mu}_0$.
   - $\boldsymbol{\Sigma}^{\text{prop}}(t) = \mathbf{P}(t)^\top (\boldsymbol{\Sigma}_0 - \text{diag}(\boldsymbol{\mu}_0))\mathbf{P}(t) + \text{diag}(\boldsymbol{\mu}^{\text{prop}}(t))$.

6. Update:

   - $\boldsymbol{\mu}^{\text{post}}(t) = \boldsymbol{\mu}^{\text{prop}}(t) + \mathbf{g}\,\delta/\sigma^2_{\bar{y}^{\text{pred}}}$.
   - $\boldsymbol{\Sigma}^{\text{post}}(t) = \boldsymbol{\Sigma}^{\text{prop}}(t) - \mathbf{g}\mathbf{g}^\top/\sigma^2_{\bar{y}^{\text{pred}}}$.

All steps use only K-vector and $K \times K$-matrix objects; no $K^2 \times K^2$ boundary covariance is ever instantiated.

11 Numerical notes and invariants

- $\boldsymbol{\Sigma}_0$ and $\boldsymbol{\Sigma}^{\text{prop}}(t)$ should be symmetric; small asymmetries from floating point should be symmetrized explicitly.
- The predictive variance $\sigma^2_{\bar{y}^{\text{pred}}}$ must be strictly positive; in practice, impose a lower bound to avoid division by zero.
- The posterior covariance $\boldsymbol{\Sigma}^{\text{post}}(t)$ is obtained by a rank-1 subtraction; numerical positive-semidefiniteness violations can be mitigated by enforcing symmetry and clipping tiny negative eigenvalues in post-processing.
- Computational complexity: matrix–matrix multiplications are $O(K^3)$ (dominated by covariance propagation); Hadamard products and tilde expressions are $O(K^2)$.

A Pedagogical narrative (optional)

This appendix compresses the conceptual story of MacroIR; it is not needed for implementation, but can help with intuition.

A.1 Why boundary states?

The interval-averaged current of a channel depends on its entire trajectory over $[0, t]$, not just its start or end state. Directly integrating over all trajectories is intractable.

MacroIR uses the following trick:

1. Introduce boundary states (i_0, i_t).

2. For each boundary pair, precompute:

   - mean interval current $\overline{\Gamma}_{i_0 \to i_t}$,
   - variance $\overline{V}_{i_0 \to i_t}$.

3. Note that, given initial counts, channels from each i_0 split multinomially into end states with probabilities $P_{i_0 \to i_t}(t)$. The random boundary counts $N_{i_0 \to i_t}$ therefore contain all the trajectory information that matters for the interval current.

The macroscopic interval current can then be written as a linear functional of the boundary counts plus additive noise:

$$\overline{y}_{0\to t} \approx \sum_{i_0,i_t} \overline{\Gamma}_{i_0\to i_t} N_{i_0\to i_t} + \text{noise}.$$

A.2 Why the tilde operator?

Naively, the boundary count covariance is a $K^2 \times K^2$ object, which we never want to build explicitly. Instead, observe:

- The prior information lives in the state space at $t = 0$: $(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$.
- The microscopic physics over $[0, t]$ is fully captured by:
  - the transition matrix $\mathbf{P}(t)$,
  - the boundary tables $\overline{\mathbf{\Gamma}}, \overline{\mathbf{V}}$.

The tilde operator is the algebraic mechanism that:

1. *Lifts* a state-space vector (such as $\overline{\gamma}_0$) into the boundary space via the boundary matrices.
2. *Modulates* it with the transition probabilities $\mathbf{P}(t)$ and the initial covariance $\boldsymbol{\Sigma}_0$.
3. *Collapses* back to either:
   - a scalar $\widetilde{u^\top \Sigma w}$, or
   - a vector $\widetilde{u^\top \Sigma}$,

   without ever explicitly constructing the full boundary covariance.

Conceptually:

- $\widetilde{\gamma^\top \Sigma \gamma}$ is the scalar one would obtain by forming the boundary covariance and applying the quadratic form defined by the boundary current weights.
- $\widetilde{\gamma^\top \Sigma}$ is the cross-covariance between the macroscopic state at time t and the interval current.

The lift–modulate–collapse pattern is the same in both cases; only the rank of the underlying algebraic expression differs, just like comparing $v^\top A$ (vector) with $v^\top A w$ (scalar) in ordinary matrix algebra.

A.3 Why the update looks like a scalar Kalman filter

Once you have:

- a prior Gaussian state at time t, $(\boldsymbol{\mu}^{\text{prop}}(t), \boldsymbol{\Sigma}^{\text{prop}}(t))$;
- a scalar observation $\overline{y}^{\text{obs}}_{0\to t}$;
- its predictive mean and variance $\overline{y}^{\text{pred}}_{0\to t}, \sigma^2_{\overline{y}^{\text{pred}}}$;
- a cross-covariance vector $\mathbf{g}$;

you are exactly in the setting of a one-dimensional Kalman update in a K-dimensional state space:

- $\mathbf{g}$ plays the role of "measurement vector times prior covariance",
- $\sigma^2_{\overline{y}^{\text{pred}}}$ is the total effective measurement variance.

The update

$$\boldsymbol{\mu}^{\text{post}} = \boldsymbol{\mu}^{\text{prop}} + \frac{\mathbf{g}}{\sigma^2_{\overline{y}^{\text{pred}}}}\delta, \qquad \boldsymbol{\Sigma}^{\text{post}} = \boldsymbol{\Sigma}^{\text{prop}} - \frac{\mathbf{g}\mathbf{g}^\top}{\sigma^2_{\overline{y}^{\text{pred}}}},$$

is precisely the Gaussian conditioning formula for a joint Gaussian variable $(\boldsymbol{N}_{\text{ch}}(t), \overline{y}_{0\to t})$.

MacroIR's distinctive feature is not the Kalman structure itself, but that $\mathbf{g}$ and $\sigma^2_{\overline{y}^{\text{pred}}}$ are computed from *interval physics* via boundary matrices and the unified tilde operator, rather than from a naive instant-state observation model.