Online Appendices

F. Explicit solutions for 1×2, 2×1 and 2×2 junctions

In this section we present the explicit solutions used for the dynamics of the optimization problem and in the software implementation. We restrict our attention to 1×2, 2×1, and 2×2 junctions, since most road networks can be modeled using only these junction types.

(1×2) diverge junction

The explicit solution was already derived in Section D.1 for the general $(1 \times n)$ case.

(2×1) merge

Let i_1 be one incoming cell, i_2 be the other incoming cell and j be the outgoing cell. As shown in Figure F.1a, we distinguish 3 cases based on where the priority vector intersects the demand constraints. The cases are $\frac{P_1}{P_2} > \left(\frac{P_1}{P_2}\right)_{max}$, $\left(\frac{P_1}{P_2}\right)_{min} \leq \frac{P_1}{P_2} \leq \left(\frac{P_1}{P_2}\right)_{max}$ and $\frac{P_1}{P_2} < \left(\frac{P_1}{P_2}\right)_{min}$, where $\left(\frac{P_1}{P_2}\right)_{max} = \frac{\delta_{i_1}}{f_j^{\text{in}} - \delta_{i_1}}$ and $\left(\frac{P_1}{P_2}\right)_{min} = \frac{f_j^{\text{in}} - \delta_{i_2}}{\delta_{i_2}}$.

In call cases, the flow into the outgoing cell is the minimum of the total supply and demand values.

$$f_j^{\text{in}}(k) = \min\left(\delta_{i_1}(k) + \delta_{i_2}(k), \sigma_j(k)\right) \tag{F.1}$$

The flow out of incoming cells depends on the priority vector and is given by the solution to the optimization problem in equation (D.5).

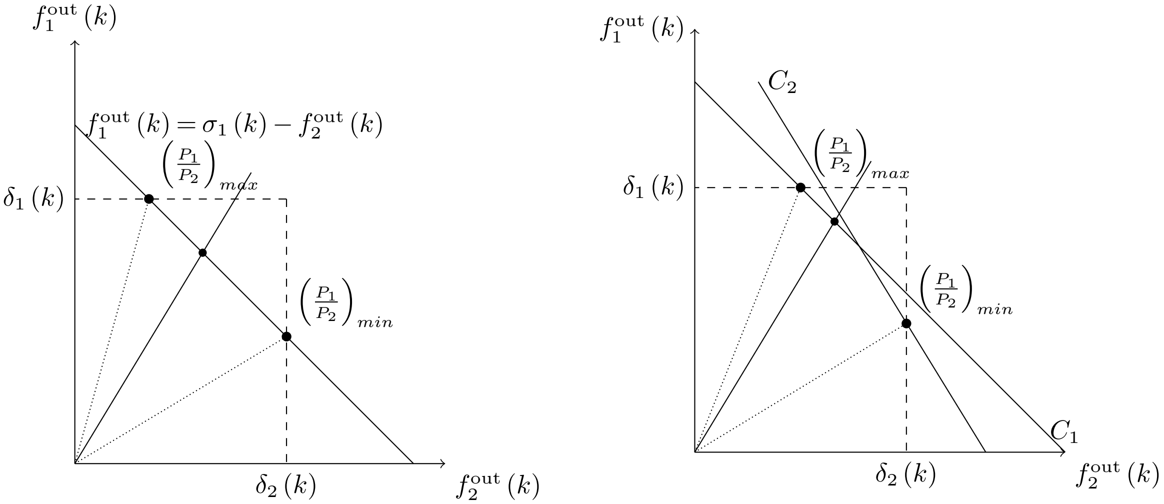
$$\begin{aligned} f_{i_1}^{\text{out}}(k) &= \begin{cases} \delta_{i_1}(k) & \text{if } P_{i_1}\left(f_j^{\text{in}}(k) - \delta_{i_1}(k)\right) > \delta_{i_1}(k) P_{i_2} \\ f_j^{\text{in}}(k) - \delta_{i_2}(k) & \text{if } P_{i_2}\left(f_j^{\text{in}}(k) - \delta_{i_2}(k)\right) > \delta_{i_2}(k) P_{i_1} \\ P_{i_1} f_j^{\text{in}}(k) & \text{otherwise} \end{cases} \\ f_{i_2}^{\text{out}}(k) &= f_j^{\text{in}}(k) - f_{i_1}^{\text{out}}(k) \end{aligned} \tag{F.2}$$

The flow out by commodity can then be computed as follows.

$$f_{i,c}^{\text{out}}(k) = \frac{\rho_{i,c}(k)}{\rho_i(k)} f_i^{\text{out}}(k) \qquad \forall i \in \{i_1, i_2\} \tag{F.3}$$

(2×2) merge and diverge

Let i_1, i_2 be the incoming cells and j_1, j_2 be the outgoing cells. To simplify the notation, we use the following shorthand:



(a) 2×1 junction

(b) 2×2 junction

Figure F.1 Graph displaying the constraints for different junctions. A similar illustration appears in Daganzo (1995).

- drop the time index k
- $\delta_1 = \delta_{i_1}$, $\delta_2 = \delta_{i_2}$
- $\sigma_1 = \sigma_{j_1}$, $\sigma_1 = \sigma_{j_2}$
- $P_1 = P_{i_1}$, $P_2 = P_{i_2}$

The aggregate split ratios are computed as follows.

$$\beta_{ij}(k) = \frac{1}{\rho_i(k)} \sum_{c=1}^{C} \rho_{i,c}(k)\, \beta_{ij,c}(k) \qquad \forall (i,j) \in \{1,2\} \times \{1,2\} \tag{F.4}$$

As shown in Figure F.1b, we once again distinguish 3 cases based on where the priority vector intersects the demand constraints. The cases are $\frac{P_1}{P_2} > \left(\frac{P_1}{P_2}\right)_{max}$, $\left(\frac{P_1}{P_2}\right)_{min} \leq \frac{P_1}{P_2} \leq \left(\frac{P_1}{P_2}\right)_{max}$ and $\frac{P_1}{P_2} < \left(\frac{P_1}{P_2}\right)_{min}$.

The values of $\left(\frac{P_1}{P_2}\right)_{max}$ (and $\left(\frac{P_1}{P_2}\right)_{min}$) can be obtained by plugging substituting δ_1 (and resp. δ_2) for f_1^{out} (and resp. f_1^{out}) in the equations C_j for the supply constraints.

$$C_j : \beta_{1j} f_1^{\text{out}} + \beta_{2j} f_2^{\text{out}} = \sigma_j \tag{F.5}$$

Thus, we obtain:

$$\left(\frac{P_1}{P_2}\right)_{max} = \frac{\delta_1}{\min\left(\delta_2, \frac{\sigma_1 - \beta_{11}\delta_1}{\beta_{21}}, \frac{\sigma_2 - \beta_{12}\delta_1}{\beta_{22}}\right)} \tag{F.6}$$

$$\left(\frac{P_1}{P_2}\right)_{min} = \frac{\min\left(\delta_1, \frac{\sigma_1 - \beta_{21}\delta_2}{\beta_{11}}, \frac{\sigma_2 - \beta_{22}\delta_2}{\beta_{12}}\right)}{\delta_2} \tag{F.7}$$

We can then compute the flow out of incoming cells using the optimization problem in equation (D.7). Since the problem is symmetric in i_1 and i_2, we just solve it for $i_1 = 1$.

- If $\frac{P_1}{P_2} > \left(\frac{P_1}{P_2}\right)_{max}$, the solution is the intersection of $f_1^{\text{out}} = \delta_1$ and the most constraining supply constraint (C_1 in Figure F.1b), and results in the trivial solution of $f_1^{\text{out}} = \delta_1$.
- If $\frac{P_1}{P_2} < \left(\frac{P_1}{P_2}\right)_{min}$, the solution is the intersection of $f_2^{\text{out}} = \delta_2$ and the most constraining supply constraint (C_2 in Figure F.1b), and therefore we obtain:
$f_1^{\text{out}} = \min\left(\delta_1, \frac{\sigma_1 - \beta_{21}\delta_2}{\beta_{11}}, \frac{\sigma_2 - \beta_{22}\delta_2}{\beta_{12}}\right)$
- If $\left(\frac{P_1}{P_2}\right)_{min} \leq \frac{P_1}{P_2} \leq \left(\frac{P_1}{P_2}\right)_{max}$, the solution lies at the point where the priority vector intersects the most constraining supply constraint ((C_2 in Figure F.1b)), and therefore we obtain:
$f_1^{\text{out}} = \min\left(\frac{P_1\sigma_1}{P_1\beta_{11} + P_2\beta_{21}}, \frac{P_1\sigma_2}{P_1\beta_{12} + P_2\beta_{22}}\right)$

This gives us the explicit following explicit solution for f_1^{out} at a 2 × 2 junction.

$$f_1^{\text{out}} = \begin{cases} \delta_1 & \text{if } \frac{P_1}{P_2} > \frac{\delta_1}{\min\left(\delta_2, \frac{\sigma_1 - \beta_{11}\delta_1}{\beta_{21}}, \frac{\sigma_2 - \beta_{12}\delta_1}{\beta_{22}}\right)} \\ \min\left(\delta_1, \frac{\sigma_1 - \beta_{21}\delta_2}{\beta_{11}}, \frac{\sigma_2 - \beta_{22}\delta_2}{\beta_{12}}\right) & \text{if } \frac{P_1}{P_2} < \frac{\min\left(\delta_1, \frac{\sigma_1 - \beta_{21}\delta_2}{\beta_{11}}, \frac{\sigma_2 - \beta_{22}\delta_2}{\beta_{12}}\right)}{\delta_2} \\ \min\left(\frac{P_1\sigma_1}{P_1\beta_{11} + P_2\beta_{21}}, \frac{P_1\sigma_2}{P_1\beta_{12} + P_2\beta_{22}}\right) & \text{otherwise} \end{cases} \tag{F.8}$$

f_2^{out} is obtained by symmtery.

Finally, we can now compute the flow out of incoming cells by commodity.

$$f_{i,c}^{\text{out}} = \frac{\rho_{i,k}}{\rho_i} f_i^{\text{out}} \qquad \forall i \in \{1,2\},\ \forall c \in C \tag{F.9}$$

G. Computing the partial derivatives of the constraints with respect to the state variables ($\frac{\partial}{\partial x}$)

We first iterate through the three classes of variables density, outflow and inflow. All unlisted derivatives evaluate to zero.

Commodity density $\rho_{i,c}(k)$ from equations (H1a, H1b, H1c, H1d))

$$\frac{\partial \rho_{i,c}(k)}{\partial \rho_{i,c}(k-1)} = 1, \qquad \forall c \in \mathcal{C},\ \forall i \in \mathcal{A} \setminus \mathcal{B}, \qquad \forall k \in [\![1, T_f]\!] \tag{G.1}$$

$$\frac{\partial \rho_{i,c}(k)}{\partial f_{i,c}^{\text{in}}(k-1)} = \frac{\Delta t}{L_i}, \qquad \forall c \in \mathcal{C},\ \forall i \in \mathcal{A} \setminus \mathcal{B}, \qquad \forall k \in [\![1, T_f]\!] \tag{G.2}$$

$$\frac{\partial \rho_{i,c}(k)}{\partial f_{i,c}^{\text{out}}(k-1)} = -\frac{\Delta t}{L_i}, \qquad \forall c \in \mathcal{C},\ \forall i \in \mathcal{A} \setminus \mathcal{S}, \qquad \forall k \in [\![1, T_f]\!] \tag{G.3}$$

Flow in $f_{i,c}^{\text{in}}$ from equation (H6)

$$\frac{\partial f_{j,c}^{\text{in}}}{\partial f_{i,c}^{\text{out}}} = \beta_{ij,c} \qquad \forall i \in \mathcal{J}_z^{\text{in}},\ \forall j \in \mathcal{J}_z^{\text{out}},\ \forall z \in \mathcal{J} \qquad \forall k \in [\![1, T_f - 1]\!] \tag{G.4}$$

Computing the partial derivatives of the flow out $f_{i,c}^{\text{out}}$ is requires a much more involved process. We begin by computing the following intermediate partial derivatives:

- Computing $\frac{\partial}{\partial \rho_{i,c}(k)}\left(\frac{\rho_{i,c}(k)\delta_i(k)}{\rho_i(k)}\right)$:

From equations (H2a, H2b),

$$\delta_i(k) = \begin{cases} \min\left(F_i, v_i\rho_i(k)\right) & \forall i \in \mathcal{A}\setminus(\mathcal{B}\cup\mathcal{S}),\ \forall k \in [\![0, T_f]\!] \\ \min\left(F_i, \frac{\rho_i(k)L_i}{\Delta t}\right) & \forall i \in \mathcal{B},\ \forall k \in [\![0, T_f]\!] \end{cases} \tag{G.5}$$

which gives the following equations:

$$\frac{\rho_{i,c}(k)}{\rho_i(k)}\delta_i(k) = \begin{cases} \min\left(\frac{\rho_{i,c}(k)}{\rho_i(k)}F_i, \rho_{i,c}(k)\, v_i\right) & \forall i \in \mathcal{A}\setminus(\mathcal{B}\cup\mathcal{S}),\ \forall k \in [\![0, T_f]\!] \\ \min\left(\frac{\rho_{i,c}(k)}{\rho_i(k)}F_i, \frac{\rho_{i,c}(k)L_i}{\Delta t}\right) & \forall i \in \mathcal{B},\ \forall k \in [\![0, T_f]\!] \end{cases} \tag{G.6}$$

Using equation (1),

$\forall i \in \mathcal{A}\setminus(\mathcal{B}\cup\mathcal{S}),\ \forall k \in [\![0, T_f]\!]$

$$\frac{\partial}{\partial \rho_{i,c}(k)}\left(\frac{\rho_{i,c}(k)}{\rho_i(k)}\delta_i(k)\right) = \begin{cases} \frac{\left(\rho_i(k)-\rho_{i,c}(k)\right)}{\rho_i(k)^2}F_i & \text{if } F_i < v_i\rho_i(k) \\ v_i & \text{otherwise} \end{cases} \tag{G.7}$$

$\forall i \in \mathcal{B},\ \forall k \in [\![0, T_f]\!]$

$$\frac{\partial}{\partial \rho_{i,c}(k)}\left(\frac{\rho_{i,c}(k)}{\rho_i(k)}\delta_i(k)\right) = \begin{cases} \frac{\left(\rho_i(k)-\rho_{i,c}(k)\right)}{\rho_i(k)^2}F_i & \text{if } F_i < \frac{L_i}{\Delta t}\rho_i(k) \\ \frac{L_i}{\Delta t} & \text{otherwise} \end{cases} \tag{G.8}$$

REMARK 5. If $\rho_i(k) = 0$, then $F_i > \frac{L_i}{\Delta t}\rho_i(k)$ or $F_i > v_i\rho_i(k)$, so the derivatives are well defined.

- Computing $\frac{\partial}{\partial \rho_{i,c'}(k)}\left(\frac{\rho_{i,c}(k)\delta_i(k)}{\rho_i(k)}\right)$: (Note the two different commodities c and c'.)

$\forall i \in \mathcal{A}\setminus(\mathcal{B}\cup\mathcal{S}),\ \forall k \in [\![0, T_f]\!]$

$$\frac{\partial}{\partial \rho_{i,c'}(k)}\left(\frac{\rho_{i,c}(k)}{\rho_i(k)}\delta_i(k)\right) = \begin{cases} \frac{-\rho_{i,c}(k)}{\rho_i(k)^2}F_i & \text{if } F_i < v_i\rho_i(k) \\ 0 & \text{otherwise} \end{cases} \tag{G.9}$$

$\forall i \in \mathcal{B},\ \forall k \in [\![0, T_f]\!]$

$$\frac{\partial}{\partial \rho_{i,c'}(k)}\left(\frac{\rho_{i,c}(k)}{\rho_i(k)}\delta_i(k)\right) = \begin{cases} \frac{-\rho_{i,c}(k)}{\rho_i(k)^2}F_i & \text{if } F_i < \frac{L_i}{\Delta t}\rho_i(k) \\ 0 & \text{otherwise} \end{cases} \tag{G.10}$$

REMARK 6. If $\rho_i(k) = 0$, then $F_i > \frac{L_i}{\Delta t}\rho_i(k)$ or $F_i > v_i\rho_i(k)$, so the derivatives are well defined.

- Computing $\frac{\partial}{\partial \rho_{i,c}(k)}\left(\frac{\rho_{i,c}(k)\sigma_j(k)}{\rho_i(k)}\right)$ and $\frac{\partial}{\partial \rho_{i,c'}(k)}\left(\frac{\rho_{i,c}(k)\sigma_j(k)}{\rho_i(k)}\right)$ when $i \neq j$:

Note that $\sigma_j(k)$ does not contain $\rho_i(k)$ terms.

$$\frac{\partial}{\partial \rho_{i,c}(k)}\left(\frac{\rho_{i,c}(k)}{\rho_i(k)}\sigma_j(k)\right) = \frac{\left(\rho_i(k)-\rho_{i,c}(k)\right)}{\rho_i(k)^2}\sigma_j(k) \tag{G.11}$$

$$\frac{\partial}{\partial \rho_{i,c'}(k)}\left(\frac{\rho_{i,c}(k)}{\rho_i(k)}\sigma_j(k)\right) = \frac{-\rho_{i,c}(k)}{\rho_i(k)^2}\sigma_j(k) \tag{G.12}$$

Remark 7. This partial derivative is only needed in cases where the junction is strictly supply constrained and $\rho_i(k) > 0$, so we can ignore the fact that the derivative is undefined at $\rho_i(k) = 0$.

- Computing $\frac{\partial}{\partial \rho_{j,c'}(k)} \left(\frac{\rho_{i,c}(k)\sigma_j(k)}{\rho_i(k)} \right)$:

From equations (H3a, H3b),

$$\sigma_j(k) = \begin{cases} \min\left(F_i, w_j\left(\rho_j^{\text{jam}} - \rho_j(k)\right)\right) & \forall j \in \mathcal{A} \setminus (\mathcal{B} \cup \mathcal{S}),\ \forall k \in [\![0, T_f]\!] \\ F_j & \forall j \in \mathcal{S},\ \forall k \in [\![0, T_f]\!] \end{cases} \tag{G.13}$$

$$\frac{\rho_{i,c}(k)}{\rho_i(k)}\sigma_j(k) = \begin{cases} \min\left(\frac{\rho_{i,c}(k)}{\rho_i(k)}F_j, \frac{\rho_{i,c}(k)}{\rho_i(k)}w_j\left(\rho_j^{\text{jam}} - \rho_j(k)\right)\right) & \forall i \in \mathcal{A} \setminus (\mathcal{B} \cup \mathcal{S}),\ \forall k \in [\![0, T_f]\!] \\ \frac{\rho_{i,c}(k)}{\rho_i(k)}F_j & \forall i \in \mathcal{S},\ \forall k \in [\![0, T_f]\!] \end{cases} \tag{G.14}$$

$\forall i \in \mathcal{A} \setminus (\mathcal{B} \cup \mathcal{S}),\ \forall k \in [\![0, T_f]\!]$

$$\frac{\partial}{\partial \rho_{j,c'}(k)} \left(\frac{\rho_{i,c}(k)}{\rho_i(k)}\sigma_j(k) \right) = \begin{cases} 0 & \text{if } F_j < w_j\left(\rho_j^{\text{jam}} - \rho_j(k)\right) \\ -\frac{\rho_{i,c}(k)}{\rho_i(k)}w_j & \text{otherwise} \end{cases} \tag{G.15}$$

$\forall i \in \mathcal{S},\ \forall k \in [\![0, T_f]\!]$

$$\frac{\partial}{\partial \rho_{j,c'}(k)} \left(\frac{\rho_{i,c}(k)}{\rho_i(k)}\sigma_j(k) \right) = 0 \tag{G.16}$$

Remark 8. This partial derivative is only needed in cases where the junction is strictly supply constrained and $\rho_i(k) > 0$, so we can ignore the fact that the derivative is undefined at $\rho_i(k) = 0$.

- Computing $\frac{\partial}{\partial \rho_{i,c}(k)} \left(\frac{\rho_{i,c}(k)\sigma_j(k)}{\rho_i(k)\beta_{ij}(k)} \right)$:

From equation (H4),

$$\beta_{ij}(k) = \frac{1}{\rho_i(k)} \sum_{c' \in \mathcal{C}} \rho_{i,c'}(k)\, \beta_{ij,c'}(k) \qquad \forall k \in [\![0, T_f]\!] \tag{G.17}$$

Let $\kappa_{ij}(k) = \sum_{c' \in \mathcal{C}} \rho_{i,c'}(k)\, \beta_{ij,c'}(k)$

$$\frac{\rho_{i,c}(k)}{\rho_i(k)} \frac{\sigma_j(k)}{\beta_{ij}(k)} = \frac{\rho_{i,c}(k)\, \sigma_j(k)}{\kappa_{ij}(k)} \tag{G.18}$$

$$\frac{\partial}{\partial \rho_{i,c}(k)} \left(\frac{\rho_{i,c}(k)}{\rho_i(k)} \frac{\sigma_j(k)}{\beta_{ij}(k)} \right) = \frac{\kappa_{ij}(k)\sigma_j(k) - \rho_{i,c}(k)\, \sigma_j(k)\, \beta_{ij,c}(k)}{\kappa_{ij}(k)^2} \tag{G.19}$$

Remark 9. This partial derivative is only needed in cases where the junction is strictly supply constrained and $\rho_i(k) > 0$, so we can ignore the fact that the derivative is undefined at $\rho_i(k) = 0$.

- Computing $\frac{\partial}{\partial \rho_{i,c'}(k)} \left(\frac{\rho_{i,c}(k)\sigma_j(k)}{\rho_i(k)\beta_{ij}(k)} \right)$:

$$\frac{\partial}{\partial \rho_{i,c'}(k)} \left(\frac{\rho_{i,c}(k)}{\rho_i(k)} \frac{\sigma_j(k)}{\beta_{ij}(k)} \right) = \frac{-\rho_{i,c}(k)\, \sigma_j(k)\, \beta_{ij,c'}(k)}{\kappa_{ij}(k)^2} \tag{G.20}$$

REMARK 10. The $\rho_i(k) = 0$ condition is just as in the previous case.

- Computing $\frac{\partial}{\partial \rho_{j,c'}(k)} \left(\frac{\rho_{i,c}(k)\sigma_j(k)}{\rho_i(k)\beta_{ij}(k)} \right)$:

$$\frac{\partial}{\partial \rho_{j,c'}(k)} \left(\frac{\rho_{i,c}(k)}{\rho_i(k)} \frac{\sigma_j(k)}{\beta_{ij}(k)} \right) = \frac{1}{\beta_{ij}(k)} \frac{\partial}{\partial \rho_{i,c'}(k)} \left(\frac{\rho_{i,c}(k)\sigma_j(k)}{\rho_i(k)} \right) \tag{G.21}$$

which can then be simplified using equations (G.15, G.16).

Now we can proceed to computing the partial derivatives of $f^{\text{out}}_{i,c}$.

DEFINITION 19 (DEMAND-CONSTRAINED JUNCTION). A junction is demand-constrained if the flow through the junction is limited by the incoming flow of cell i. We denote this condition by $DC(i)$.

DEFINITION 20 (SUPPLY-CONSTRAINED JUNCTION). A junction is supply-constrained if the flow through the junction is limited by the outgoing flow into some outgoing cell j. We denote this condition by $SC(j)$.

Solution for 1×2 junctions

The solutions to all the partial derivatives that appear in the expressions below have already been solved explicitly.

From equation (H5a),

$$f^{\text{out}}_{i,c} = \frac{\rho_{i,c}}{\rho_i} \min\left(\left\{ \frac{\sigma_j(k)}{\beta_{ij}(k)},\ \forall j \in \mathcal{J}^{\text{out}}_z \mid \beta_{ij}(k) > 0 \right\}, \delta_i(k) \right) \qquad \forall z \in \mathcal{J}_{1\times n},\ \forall i \in \mathcal{J}^{\text{in}}_z \tag{G.22}$$

$$\frac{\partial f^{\text{out}}_{i,c}}{\partial \rho_{i,c}(k)} = \begin{cases} \frac{\partial}{\partial \rho_{i,c}(k)} \left(\frac{\rho_{i,c}(k)\delta_i(k)}{\rho_i(k)} \right) & \text{if } DC(i) \\ \frac{\partial}{\partial \rho_{i,c}(k)} \left(\frac{\rho_{i,c}(k)}{\rho_i(k)} \frac{\sigma_i(k)}{\beta_{ij}(k)} \right) & \text{if } SC(j) \end{cases} \tag{G.23}$$

$$\frac{\partial f^{\text{out}}_{i,c'}}{\partial \rho_{i,c}(k)} = \begin{cases} \frac{\partial}{\partial \rho_{i,c}(k)} \left(\frac{\rho_{i,c'}(k)\delta_i(k)}{\rho_i(k)} \right) & \text{if } DC(i) \\ \frac{\partial}{\partial \rho_{i,c}(k)} \left(\frac{\rho_{i,c'}(k)}{\rho_i(k)} \frac{\sigma_i(k)}{\beta_{ij}(k)} \right) & \text{if } SC(j) \end{cases} \tag{G.24}$$

$$\frac{\partial f^{\text{out}}_{i,c}}{\partial \rho_{j,c'}(k)} = \begin{cases} 0 & \text{if } DC(i) \\ \frac{\partial}{\partial \rho_{j,c'}(k)} \left(\frac{\rho_{i,c}(k)}{\rho_i(k)} \frac{\sigma_i(k)}{\beta_{ij}(k)} \right) & \text{if } SC(j) \end{cases} \tag{G.25}$$

REMARK 11. It is important to note that these derivatives are undefined if the junction is both supply and demand-constrained. However, this can only occur if the density of the cell is exactly equal to the value at which the demand and supply constraints meet. This is extremely unlikely in practice with floating point numerical operations. In the rare event that it does occur, we assume that the junction is supply-constrained.

Solution for 2×1 junctions

The solutions to all the partial derivatives that appear in the expressions below have already been solved explicitly.

From equation (H5b)

$$f_{i,c}^{\text{out}} = \frac{\rho_{i,c}}{\rho_i} \begin{cases} \delta_i & \text{if } P_i \left(\min\left(\delta_i + \delta_{\underline{i}}, \sigma_j\right) - \delta_i\right) > \delta_i P_{\underline{i}} \\ \min\left(\delta_i + \delta_{\underline{i}}, \sigma_j\right) - \delta_{\underline{i}} & \text{if } P_{\underline{i}} \left(\min\left(\delta_i + \delta_{\underline{i}}, \sigma_j\right) - \delta_{\underline{i}}\right) > \delta_{\underline{i}} P_i \\ P_i \min\left(\delta_i + \delta_{\underline{i}}, \sigma_j\right) & \text{otherwise} \end{cases} \quad \forall z \in \mathcal{J}_{2\times 1},\ \forall i \in \mathcal{J}_z^{\text{in}} \tag{G.26}$$

case 1: $P_i \left(\min\left(\delta_i + \delta_{\underline{i}}, \sigma_j\right) - \delta_i\right) > \delta_i P_{\underline{i}}$

$$\frac{\partial f_{i,c}^{\text{out}}}{\partial \rho_{i,c}(k)} = \frac{\partial}{\partial \rho_{i,c}(k)} \left(\frac{\rho_{i,c}(k)\, \delta_i(k)}{\rho_i(k)} \right) \tag{G.27}$$

$$\frac{\partial f_{i,c'}^{\text{out}}}{\partial \rho_{i,c}(k)} = \frac{\partial}{\partial \rho_{i,c}(k)} \left(\frac{\rho_{i,c'}(k)\, \delta_i(k)}{\rho_i(k)} \right) \tag{G.28}$$

$$\frac{\partial f_{i,c'}^{\text{out}}}{\partial \rho_{j,c}(k)} = 0 \tag{G.29}$$

case 2: $P_{\underline{i}} \left(\min\left(\delta_i + \delta_{\underline{i}}, \sigma_j\right) - \delta_{\underline{i}}\right) > \delta_{\underline{i}} P_i$

$$\frac{\partial f_{i,c}^{\text{out}}}{\partial \rho_{i,c}(k)} = \begin{cases} \frac{\partial}{\partial \rho_{i,c}(k)} \left(\frac{\rho_{i,c}(k)\delta_i(k)}{\rho_i(k)} \right) & \text{if } \delta_i + \delta_{\underline{i}} < \sigma_j \\ \frac{\partial}{\partial \rho_{i,c}(k)} \left(\frac{\rho_{i,c}(k)\sigma_j(k)}{\rho_i(k)} \right) - \frac{\partial}{\partial \rho_{i,c}(k)} \left(\frac{\rho_{i,c}(k)\delta_{\underline{i}}(k)}{\rho_i(k)} \right) & \text{otherwise} \end{cases} \tag{G.30}$$

$$\frac{\partial f_{i,c}^{\text{out}}}{\partial \rho_{i,c'}(k)} = \begin{cases} \frac{\partial}{\partial \rho_{i,c'}(k)} \left(\frac{\rho_{i,c}(k)\delta_i(k)}{\rho_i(k)} \right) & \text{if } \delta_i + \delta_{\underline{i}} < \sigma_j \\ \frac{\partial}{\partial \rho_{i,c'}(k)} \left(\frac{\rho_{i,c}(k)\sigma_j(k)}{\rho_i(k)} \right) - \frac{\partial}{\partial \rho_{i,c}(k)} \left(\frac{\rho_{i,c}(k)\delta_{\underline{i}}(k)}{\rho_i(k)} \right) & \text{otherwise} \end{cases} \tag{G.31}$$

$$\frac{\partial f_{i,c}^{\text{out}}}{\partial \rho_{j,c'}(k)} = \begin{cases} 0 & \text{if } \delta_i + \delta_{\underline{i}} < \sigma_j \\ \frac{\partial}{\partial \rho_{j,c'}(k)} \left(\frac{\rho_{i,c}(k)\sigma_j(k)}{\rho_i(k)} \right) & \text{otherwise} \end{cases} \tag{G.32}$$

case 3: otherwise

$$\frac{\partial f_{i,c}^{\text{out}}}{\partial \rho_{i,c}(k)} = \begin{cases} P_i \left(\frac{\partial}{\partial \rho_{i,c}(k)} \left(\frac{\rho_{i,c}(k)\delta_i(k)}{\rho_i(k)} \right) + \frac{\partial}{\partial \rho_{i,c}(k)} \left(\frac{\rho_{i,c}(k)\delta_{\underline{i}}(k)}{\rho_i(k)} \right) \right) & \text{if } \delta_i + \delta_{\underline{i}} < \sigma_j \\ P_i \left(\frac{\partial}{\partial \rho_{i,c}(k)} \left(\frac{\rho_{i,c}(k)\sigma_j(k)}{\rho_i(k)} \right) \right) & \text{otherwise} \end{cases} \tag{G.33}$$

$$\frac{\partial f_{i,c}^{\text{out}}}{\partial \rho_{i,c'}(k)} = \begin{cases} P_i \left(\frac{\partial}{\partial \rho_{i,c'}(k)} \left(\frac{\rho_{i,c}(k)\delta_i(k)}{\rho_i(k)} \right) + \frac{\partial}{\partial \rho_{i,c}(k)} \left(\frac{\rho_{i,c}(k)\delta_{\underline{i}}(k)}{\rho_i(k)} \right) \right) & \text{if } \delta_i + \delta_{\underline{i}} < \sigma_j \\ P_i \left(\frac{\partial}{\partial \rho_{i,c'}(k)} \left(\frac{\rho_{i,c}(k)\sigma_j(k)}{\rho_i(k)} \right) \right) & \text{otherwise} \end{cases} \tag{G.34}$$

$$\frac{\partial f_{i,c}^{\text{out}}}{\partial \rho_{j,c'}(k)} = \begin{cases} 0 & \text{if } \delta_i + \delta_{\underline{i}} < \sigma_j \\ P_i \left(\frac{\partial}{\partial \rho_{j,c'}(k)} \left(\frac{\rho_{i,c}(k)\sigma_j(k)}{\rho_i(k)} \right) \right) & \text{otherwise} \end{cases} \tag{G.35}$$

Solution for 2×2 junctions

The solution for the 2×2 junctions can be obtained using a similar set of computations, but is omitted here for readability and due to length constraints.

This concludes the computation of all the partial derivatives required for computing the gradient of the system using the discrete adjoint method.

Remark 12. If we do not have closed form solutions for the junctions, it may not be possible to compute the explicit partial derivatives of the outgoing flow with respect to the partial densities of the incoming and outgoing cells of the junction. However, for any junction that cannot be solved explicitly, it is still possible to compute $\frac{\partial f_{i,c}^{\text{out}}(k)}{\partial \rho_{i',c'}(k)}$ for all $i, i' \in \mathcal{J}_z^{\text{in}} \cup \mathcal{J}_z^{\text{out}}$ and $c, c' \in \mathcal{C}$ with a finite differences method using $|\mathcal{J}_z^{\text{in}}| \cdot |\mathcal{J}_z^{\text{out}}| \cdot |\mathcal{C}|$ local simulations of just the junction dynamics (not the entire system). We can then continue to use the adjoint method while numerically differentiating these junctions that do not admit an explicit solution. This local finite differences method can still allow a very efficient computation of the gradient for heterogeneous networks with some junctions or sub-networks that contain complex dynamics.