

D Log-likelihood, Gradient and Hessian derivations

Introduction. Let us revisit our model with two parameters - inverse temperature, β , and learning rate α - that we aim to estimate. We know that the domain of these model parameters are $[0, \infty]$ and $[0, 1]$, respectively. However, given an unconstrained optimization approach (i.e., trust region), we need to perform our estimation on unconstrained parameters. Thus, our motivation behind reparameterization of parameters using x_1 and x_2 :

$$\beta = e^{x_1} \quad (\text{D.1})$$

$$\alpha = \frac{1}{1 + e^{-x_2}} \quad (\text{D.2})$$

This reparameterization allows our parameters - x_1 and x_2 - to have an unconstrained domain of $[-\infty, \infty]$ while preserving the appropriate domains of β and α . We now introduce the softmax choice function and Q-learning rule formula for choosing either machine A or machine B on trial t :

$$P(A_t) = \frac{e^{Q_{1t}}}{e^{Q_{1t}} + e^{Q_{2t}}} \quad (\text{D.3})$$

$$Q_{A_t} = Q_{A_{t-1}} + \alpha(r_{t-1} - Q_{A_{t-1}}) \quad (\text{D.4})$$

$$P(B_t) = \frac{e^{Q_{2t}}}{e^{Q_{1t}} + e^{Q_{2t}}} \quad (\text{D.5})$$

$$Q_{B_t} = Q_{B_{t-1}} + \alpha(r_{t-1} - Q_{B_{t-1}}) \quad (\text{D.6})$$

where β and α have been reparameterized and $Q_{1t} = \beta Q_{A_t}$ and $Q_{2t} = \beta Q_{B_t}$. Equations (C.3) and (C.4) represent the softmax choice function and Q-learning rule for a participants' choice of machine A, respectively. Likewise, equations (C.5) and (C.6) for machine B. **For the purpose of explaining the remaining derivations, we will perform the derivations for a particular choice (i.e., the probability a participant chooses machine A).** This means we will focus on equations (C.3) and (C.4). Let's begin by algebraically converting equation (C.4) into one indexed by 1_t (for choosing machine A on trial t):

$$\begin{aligned} Q_{A_t} &= Q_{A_{t-1}} + \alpha(r_{t-1} - Q_{A_{t-1}}) & (\text{C.4}) \\ \beta Q_{A_t} &= \beta Q_{A_{t-1}} + \alpha(\beta r_{t-1} - \beta Q_{A_{t-1}}) & (\text{multiply by } \beta) \\ Q_{1t} &= Q_{1_{t-1}} + \alpha(\beta r_{t-1} - Q_{1_{t-1}}) & (Q_{1t} = \beta Q_{A_t}) \end{aligned}$$

Hence,

$$Q_{1t} = Q_{1_{t-1}} + \alpha(\beta r_{t-1} - Q_{1_{t-1}}) \quad (\text{D.7})$$

Log-likelihood. Now that we have setup the general model we can begin performing our derivations. We will first start with the derivation of the log-likelihood for choosing machine A on a particular trial t (LL_{A_t}):

$$\begin{aligned} P(A_t) &= \frac{e^{Q_{1t}}}{e^{Q_{1t}} + e^{Q_{2t}}} & (\text{C.3}) \\ \log(P(A_t)) &= \log\left(\frac{e^{Q_{1t}}}{e^{Q_{1t}} + e^{Q_{2t}}}\right) & (\log \text{ both sides}) \\ &= \log(e^{Q_{1t}}) - \log(e^{Q_{1t}} + e^{Q_{2t}}) & (\log \text{ quotient rule}) \\ &= Q_{1t} - \log(e^{Q_{1t}} + e^{Q_{2t}}) & (\log(e^x) = x) \end{aligned}$$

Thus,

$$LL_{A_t} = \log(P(A_t)) = Q_{1t} - \log(e^{Q_{1t}} + e^{Q_{2t}}) \quad (\text{D.8})$$

Gradient. Given our log-likelihood, we are ready to compute the gradient of LL_{A_t} with respect to each of our parameters - x_1 and x_2 - as symbolized by $\frac{\partial LL_{A_t}}{\partial x_1}$ and $\frac{\partial LL_{A_t}}{\partial x_2}$, respectively :

Starting with $\frac{\partial LL_{A_t}}{\partial x_1}$:

$$\begin{aligned} LL_{A_t} &= Q_{1t} - \log(e^{Q_{1t}} + e^{Q_{2t}}) & (\text{C.8}) \\ \frac{\partial LL_{A_t}}{\partial x_1} &= \frac{\partial Q_{1t}}{\partial x_1} - \left[\frac{1}{e^{Q_{1t}} + e^{Q_{2t}}} \right] \left[\frac{\partial Q_{1t}}{\partial x_1} e^{Q_{1t}} + \frac{\partial Q_{2t}}{\partial x_1} e^{Q_{2t}} \right] & (\text{partial derivative w.r.t } x_1) \\ &= \frac{\partial Q_{1t}}{\partial x_1} - \left[P(A_t) \frac{\partial Q_{1t}}{\partial x_1} + P(B_t) \frac{\partial Q_{2t}}{\partial x_1} \right] & (\text{C.3) and (C.5)} \end{aligned}$$

from which we get

$$\frac{\partial LL_{A_t}}{\partial x_1} = \frac{\partial Q_{1_t}}{\partial x_1} - \left[P(A_t) \frac{\partial Q_{1_t}}{\partial x_1} + P(B_t) \frac{\partial Q_{2_t}}{\partial x_1} \right] \quad (\text{D.9})$$

Second, we need to solve for $\frac{\partial Q_{1_t}}{\partial x_1}$ in equation (C.9). To accomplish this we will refer to equation (C.7) and differentiate with respect to x_1 :

Solving $\frac{\partial Q_{1_t}}{\partial x_1}$:

$$\begin{aligned} Q_{1_t} &= Q_{1_{t-1}} + \alpha(\beta r_{t-1} - Q_{1_{t-1}}) & (\text{C.7}) \\ \frac{\partial Q_{1_t}}{\partial x_1} &= \frac{\partial Q_{1_{t-1}}}{\partial x_1} + \alpha r_{t-1} \frac{\partial \beta}{\partial x_1} - \alpha \frac{\partial Q_{1_{t-1}}}{\partial x_1} & (\text{partial derivative w.r.t } x_1) \\ &= (1 - \alpha) \frac{\partial Q_{1_{t-1}}}{\partial x_1} + \alpha r_{t-1} \frac{\partial \beta}{\partial x_1} & (\text{simplify using common factor}) \end{aligned}$$

Thus,

$$\frac{\partial Q_{1_t}}{\partial x_1} = (1 - \alpha) \frac{\partial Q_{1_{t-1}}}{\partial x_1} + \alpha r_{t-1} \frac{\partial \beta}{\partial x_1} \quad (\text{D.10})$$

The last step needed to evaluate equation (C.9) is to evaluate the term, $\frac{\partial \beta}{\partial x_1}$, from equation (C.10):

Getting $\frac{\partial \beta}{\partial x_1}$:

$$\begin{aligned} \beta &= e^{x_1} & (\text{C.1}) \\ \frac{\partial \beta}{\partial x_1} &= \frac{\partial e^{x_1}}{\partial x_1} & (\text{partial derivative w.r.t } x_1) \\ &= e^{x_1} & (\frac{\partial}{\partial x} e^x = e^x) \\ &= \beta & (\text{C.1}) \end{aligned}$$

Consequently,

$$\frac{\partial \beta}{\partial x_1} = \beta \quad (\text{D.11})$$

Finally, we expand equation (C.9) using equations (C.10) and (C.11) to obtain the gradient of LL_{A_t} with respect to x_1 .

We now perform a similar derivation procedure for the gradient of LL_{A_t} with respect to the other parameter, x_2 :

Starting with $\frac{\partial LL_{A_t}}{\partial x_2}$:

$$\begin{aligned} LL_{A_t} &= Q_{1_t} - \log(e^{Q_{1_t}} + e^{Q_{2_t}}) & (\text{C.8}) \\ \frac{\partial LL_{A_t}}{\partial x_2} &= \frac{\partial Q_{1_t}}{\partial x_2} - \left[\frac{1}{e^{Q_{1_t}} + e^{Q_{2_t}}} \right] \left[\frac{\partial Q_{1_t}}{\partial x_2} e^{Q_{1_t}} + \frac{\partial Q_{2_t}}{\partial x_2} e^{Q_{2_t}} \right] & (\text{partial derivative w.r.t } x_2) \\ &= \frac{\partial Q_{1_t}}{\partial x_2} - \left[P(A_t) \frac{\partial Q_{1_t}}{\partial x_2} + P(B_t) \frac{\partial Q_{2_t}}{\partial x_2} \right] & (\text{C.3 and C.5}) \end{aligned}$$

we get

$$\frac{\partial LL_{A_t}}{\partial x_2} = \frac{\partial Q_{1_t}}{\partial x_2} - \left[P(A_t) \frac{\partial Q_{1_t}}{\partial x_2} + P(B_t) \frac{\partial Q_{2_t}}{\partial x_2} \right] \quad (\text{D.12})$$

To solve for $\frac{\partial Q_{1_t}}{\partial x_2}$ in equation (C.12), we will refer to equation (C.7) and differentiate with respect to x_2 :

Solving $\frac{\partial Q_{1_t}}{\partial x_2}$:

$$\begin{aligned}
Q_{1t} &= Q_{1t-1} + \alpha(\beta r_{t-1} - Q_{1t-1}) & (\text{C.7}) \\
\frac{\partial Q_{1t}}{\partial x_2} &= \frac{\partial Q_{1t-1}}{\partial x_2} + \alpha \left[-\frac{\partial Q_{1t-1}}{\partial x_2} \right] + (\beta r_{t-1} - Q_{1t-1}) \left[\frac{\partial \alpha}{\partial x_2} \right] & (\text{partial derivative w.r.t } x_2) \\
&= (1 - \alpha) \frac{\partial Q_{1t-1}}{\partial x_2} + (\beta r_{t-1} - Q_{1t-1}) \frac{\partial \alpha}{\partial x_2} & (\text{simplify using common factor})
\end{aligned}$$

we obtain

$$\frac{\partial Q_{1t}}{\partial x_2} = (1 - \alpha) \frac{\partial Q_{1t-1}}{\partial x_2} + (\beta r_{t-1} - Q_{1t-1}) \frac{\partial \alpha}{\partial x_2} \quad (\text{D.13})$$

The last step needed to evaluate equation (C.12) is to evaluate the term, $\frac{\partial \alpha}{\partial x_2}$, from equation (C.13):

Finally, $\frac{\partial \alpha}{\partial x_2}$:

$$\begin{aligned}
\alpha &= \frac{1}{1 + e^{-x_2}} & (\text{C.2}) \\
&= (1 + e^{-x_2})^{-1} & (\text{rewritten form}) \\
\frac{\partial \alpha}{\partial x_2} &= -(1 + e^{-x_2})^{-2} (-e^{-x_2}) & (\text{partial derivative w.r.t } x_2) \\
&= (1 + e^{-x_2})^{-2} (e^{-x_2}) & (\text{divide by -1}) \\
&= (\alpha)^2 (e^{-x_2}) & (\text{since } \alpha = (1 + e^{-x_2})^{-1}) \\
&= (\alpha)^2 \left[\frac{1 - \alpha}{\alpha} \right] & (\text{solve for } e^{-x_2} \text{ in (C.2)}) \\
&= \alpha(1 - \alpha) & (\text{simplify})
\end{aligned}$$

Consequently,

$$\frac{\partial \alpha}{\partial x_2} = \alpha(1 - \alpha) \quad (\text{D.14})$$

Finally, we expand equation (C.12) using equations (C.13) and (C.14) to obtain the gradient of LL_{A_t} with respect to x_2 .

Hessian. Now that we have completed our gradient computation, we are ready to construct our Hessian matrix. Let's compute the second-order partial derivatives of LL_{A_t} with respect to each of our parameters - x_1 and x_2 - as symbolized by $\frac{\partial^2 LL_{A_t}}{\partial x_1^2}$, $\frac{\partial^2 LL_{A_t}}{\partial x_1 \partial x_2}$, $\frac{\partial^2 LL_{A_t}}{\partial x_2 \partial x_1}$ and $\frac{\partial^2 LL_{A_t}}{\partial x_2^2}$. Let's first look at our computed gradients where we replace $P(A_t)$ and $P(B_t)$ with $e^{LL_{A_t}}$ and $1 - e^{LL_{A_t}}$, respectively, from equations (C.9) and (C.12) given that we focus on participants' decision of choosing machine A:

$$\frac{\partial LL_{A_t}}{\partial x_1} = \frac{\partial Q_{1t}}{\partial x_1} - \left[e^{LL_{A_t}} \frac{\partial Q_{1t}}{\partial x_1} + (1 - e^{LL_{A_t}}) \frac{\partial Q_{2t}}{\partial x_1} \right] \quad (\text{D.15})$$

$$\frac{\partial LL_{A_t}}{\partial x_2} = \frac{\partial Q_{1t}}{\partial x_2} - \left[e^{LL_{A_t}} \frac{\partial Q_{1t}}{\partial x_2} + (1 - e^{LL_{A_t}}) \frac{\partial Q_{2t}}{\partial x_2} \right] \quad (\text{D.16})$$

Note that we can replace the probabilities with $e^{LL_{A_t}}$ because $LL_{A_t} = \log(P(A_t))$ so if we take the exponential from both sides we get $P(A_t) = e^{LL_{A_t}}$ and since $P(B_t) = 1 - P(A_t)$ we get $P(B_t) = 1 - e^{LL_{A_t}}$.

Using equations (C.15) and (C.16), we can compute the elements of the Hessian. Let's begin with the second-order direct partial derivative of LL_{A_t} w.r.t x_1 :

Solve for $\frac{\partial^2 LL_{A_t}}{\partial x_1^2}$:

$$\begin{aligned}
\frac{\partial LL_{A_t}}{\partial x_1} &= \frac{\partial Q_{1t}}{\partial x_1} - \left[e^{LL_{A_t}} \frac{\partial Q_{1t}}{\partial x_1} + (1 - e^{LL_{A_t}}) \frac{\partial Q_{2t}}{\partial x_1} \right] \\
\frac{\partial^2 LL_{A_t}}{\partial x_1^2} &= \frac{\partial^2 Q_{1t}}{\partial x_1^2} - \left[e^{LL_{A_t}} \frac{\partial^2 Q_{1t}}{\partial x_1^2} + \frac{\partial Q_{1t}}{\partial x_1} \left(\frac{\partial LL_{A_t}}{\partial x_1} e^{LL_{A_t}} \right) \right] \\
&\quad - \left[(1 - e^{LL_{A_t}}) \frac{\partial^2 Q_{2t}}{\partial x_1^2} + \frac{\partial Q_{2t}}{\partial x_1} \left(- \frac{\partial LL_{A_t}}{\partial x_1} e^{LL_{A_t}} \right) \right] \quad (\text{direct partial derivative w.r.t } x_1) \\
&= \frac{\partial^2 Q_{1t}}{\partial x_1^2} - \left[e^{LL_{A_t}} \frac{\partial^2 Q_{1t}}{\partial x_1^2} + (1 - e^{LL_{A_t}}) \frac{\partial^2 Q_{2t}}{\partial x_1^2} \right] \\
&\quad - \frac{\partial LL_{A_t}}{\partial x_1} e^{LL_{A_t}} \left(\frac{\partial Q_{1t}}{\partial x_1} - \frac{\partial Q_{2t}}{\partial x_1} \right) \quad (\text{expand and simplify})
\end{aligned} \tag{C.15}$$

resulting in

$$\frac{\partial^2 LL_{A_t}}{\partial x_1^2} = \frac{\partial^2 Q_{1t}}{\partial x_1^2} - \left[e^{LL_{A_t}} \frac{\partial^2 Q_{1t}}{\partial x_1^2} + (1 - e^{LL_{A_t}}) \frac{\partial^2 Q_{2t}}{\partial x_1^2} \right] - \frac{\partial LL_{A_t}}{\partial x_1} e^{LL_{A_t}} \left(\frac{\partial Q_{1t}}{\partial x_1} - \frac{\partial Q_{2t}}{\partial x_1} \right) \tag{D.17}$$

Now, we need to solve for $\frac{\partial^2 Q_{1t}}{\partial x_1^2}$ in equation (C.17). To accomplish this we will refer to equation (C.10) and differentiate with respect to x_1 :

Solve for $\frac{\partial^2 Q_{1t}}{\partial x_1^2}$:

$$\begin{aligned}
\frac{\partial Q_{1t}}{\partial x_1} &= (1 - \alpha) \frac{\partial Q_{1t-1}}{\partial x_1} + \alpha r_{t-1} \frac{\partial \beta}{\partial x_1} \\
\frac{\partial^2 Q_{1t}}{\partial x_1^2} &= (1 - \alpha) \frac{\partial^2 Q_{1t-1}}{\partial x_1^2} + \alpha r_{t-1} \beta \quad (\text{direct partial derivative w.r.t } x_1)
\end{aligned} \tag{C.10}$$

resulting in

$$\frac{\partial^2 Q_{1t}}{\partial x_1^2} = (1 - \alpha) \frac{\partial^2 Q_{1t-1}}{\partial x_1^2} + \alpha r_{t-1} \beta \tag{D.18}$$

Finally, we expand equation (C.17) using equation (C.22) to obtain the second-order direct partial derivative of LL_{A_t} with respect to x_1 .

We will now derive the remaining Hessian components - $\frac{\partial^2 LL_{A_t}}{\partial x_1 \partial x_2}$, $\frac{\partial^2 LL_{A_t}}{\partial x_2 \partial x_1}$ and $\frac{\partial^2 LL_{A_t}}{\partial x_2^2}$.

Solve for $\frac{\partial^2 LL_{A_t}}{\partial x_1 \partial x_2}$:

$$\begin{aligned}
\frac{\partial^2 LL_{A_t}}{\partial x_1 \partial x_2} &= \frac{\partial^2 Q_{1t}}{\partial x_1 \partial x_2} - \left[e^{LL_{A_t}} \frac{\partial^2 Q_{1t}}{\partial x_1 \partial x_2} + \frac{\partial Q_{1t}}{\partial x_1} \left(\frac{\partial LL_{A_t}}{\partial x_2} e^{LL_{A_t}} \right) \right] \\
&\quad - \left[(1 - e^{LL_{A_t}}) \frac{\partial^2 Q_{2t}}{\partial x_1 \partial x_2} + \frac{\partial Q_{2t}}{\partial x_1} \left(- \frac{\partial LL_{A_t}}{\partial x_2} e^{LL_{A_t}} \right) \right] \quad (\text{cross partial derivative of (C.16) of } x_2 \text{ w.r.t } x_1)
\end{aligned}$$

resulting in

$$\frac{\partial^2 LL_{A_t}}{\partial x_1 \partial x_2} = \frac{\partial^2 Q_{1t}}{\partial x_1 \partial x_2} - \left[e^{LL_{A_t}} \frac{\partial^2 Q_{1t}}{\partial x_1 \partial x_2} + (1 - e^{LL_{A_t}}) \left(\frac{\partial^2 Q_{2t}}{\partial x_1 \partial x_2} \right) \right] - \frac{\partial LL_{A_t}}{\partial x_2} e^{LL_{A_t}} \left(\frac{\partial Q_{1t}}{\partial x_1} - \frac{\partial Q_{2t}}{\partial x_1} \right) \tag{D.19}$$

Now, we need to solve for $\frac{\partial^2 Q_{1t}}{\partial x_1 \partial x_2}$ in equation (C.19). To accomplish this we will refer to equation (C.10) and differentiate with respect to x_1 :

Solve for $\frac{\partial^2 Q_{1t}}{\partial x_1 \partial x_2}$:

$$\begin{aligned}
\frac{\partial Q_{1t}}{\partial x_1} &= (1-\alpha) \frac{\partial Q_{1t-1}}{\partial x_1} + \alpha r_{t-1} \frac{\partial \beta}{\partial x_1} & (C.10) \\
\frac{\partial^2 Q_{1t}}{\partial x_1 \partial x_2} &= (1-\alpha) \frac{\partial^2 Q_{1t-1}}{\partial x_1 \partial x_2} - \frac{\partial \alpha}{\partial x_2} \left(\frac{\partial Q_{1t-1}}{\partial x_1} \right) + \frac{\partial \alpha}{\partial x_2} r_{t-1} \beta & (\text{cross partial derivative of } x_2 \text{ w.r.t } x_1) \\
&= (1-\alpha) \frac{\partial^2 Q_{1t-1}}{\partial x_1 \partial x_2} - (\alpha(1-\alpha)) \frac{\partial Q_{1t-1}}{\partial x_1} + (\alpha(1-\alpha)) r_{t-1} \beta & (\frac{\partial \alpha}{\partial x_2} = \alpha(1-\alpha))
\end{aligned}$$

resulting in

$$\frac{\partial^2 Q_{1t}}{\partial x_1 \partial x_2} = (1-\alpha) \frac{\partial^2 Q_{1t-1}}{\partial x_1 \partial x_2} - (\alpha(1-\alpha)) \left[\frac{\partial Q_{1t-1}}{\partial x_1} - r_{t-1} \beta \right] \quad (D.20)$$

Finally, we expand equation (C.19) using equation (C.20) to obtain the second-order cross partial derivative of LL_{A_t} of x_2 with respect to x_1 .

Solve for $\frac{\partial^2 LL_{A_t}}{\partial x_2^2}$:

$$\begin{aligned}
\frac{\partial LL_{A_t}}{\partial x_2} &= \frac{\partial Q_{1t}}{\partial x_2} - \left[e^{LL_{A_t}} \frac{\partial Q_{1t}}{\partial x_2} + (1 - e^{LL_{A_t}}) \frac{\partial Q_{2t}}{\partial x_2} \right] & (C.16) \\
\frac{\partial^2 LL_{A_t}}{\partial x_2^2} &= \frac{\partial^2 Q_{1t}}{\partial x_2^2} - \left[e^{LL_{A_t}} \frac{\partial^2 Q_{1t}}{\partial x_2^2} + \frac{\partial Q_{1t}}{\partial x_2} \left(\frac{\partial LL_{A_t}}{\partial x_2} e^{LL_{A_t}} \right) \right] \\
&\quad - \left[(1 - e^{LL_{A_t}}) \frac{\partial^2 Q_{2t}}{\partial x_2^2} + \frac{\partial Q_{2t}}{\partial x_2} \left(- \frac{\partial LL_{A_t}}{\partial x_2} e^{LL_{A_t}} \right) \right] & (\text{direct partial derivative w.r.t } x_2) \\
&= \frac{\partial^2 Q_{1t}}{\partial x_2^2} - \left[e^{LL_{A_t}} \frac{\partial^2 Q_{1t}}{\partial x_2^2} + (1 - e^{LL_{A_t}}) \frac{\partial^2 Q_{2t}}{\partial x_2^2} \right] \\
&\quad - \frac{\partial LL_{A_t}}{\partial x_2} e^{LL_{A_t}} \left(\frac{\partial Q_{1t}}{\partial x_2} - \frac{\partial Q_{2t}}{\partial x_2} \right) & (\text{expand and simplify})
\end{aligned}$$

resulting in

$$\frac{\partial^2 LL_{A_t}}{\partial x_2^2} = \frac{\partial^2 Q_{1t}}{\partial x_2^2} - \left[e^{LL_{A_t}} \frac{\partial^2 Q_{1t}}{\partial x_2^2} + (1 - e^{LL_{A_t}}) \frac{\partial^2 Q_{2t}}{\partial x_2^2} \right] - \frac{\partial LL_{A_t}}{\partial x_2} e^{LL_{A_t}} \left(\frac{\partial Q_{1t}}{\partial x_2} - \frac{\partial Q_{2t}}{\partial x_2} \right) \quad (D.21)$$

Now, we need to solve for $\frac{\partial^2 Q_{1t}}{\partial x_2^2}$ in equation (C.21). To accomplish this we will refer to equation (C.13) and differentiate with respect to x_2 :

Solve for $\frac{\partial^2 Q_{1t}}{\partial x_2^2}$:

$$\begin{aligned}
\frac{\partial Q_{1t}}{\partial x_2} &= (1-\alpha) \frac{\partial Q_{1t-1}}{\partial x_2} + (\beta r_{t-1} - Q_{1t-1}) \frac{\partial \alpha}{\partial x_2} & (C.13) \\
\frac{\partial^2 Q_{1t}}{\partial x_2^2} &= (1-\alpha) \frac{\partial^2 Q_{1t-1}}{\partial x_2^2} + \left(- \frac{\partial \alpha}{\partial x_2} \right) \frac{\partial Q_{1t-1}}{\partial x_2} \\
&\quad + (\beta r_{t-1} - Q_{1t-1}) \frac{\partial^2 \alpha}{\partial x_2^2} + \left(- \frac{\partial Q_{1t-1}}{\partial x_2} \right) \frac{\partial \alpha}{\partial x_2} & (\text{direct partial derivative w.r.t } x_2) \\
&= (1-\alpha) \frac{\partial^2 Q_{1t-1}}{\partial x_2^2} - 2(\alpha(1-\alpha)) \frac{\partial Q_{1t-1}}{\partial x_2} \\
&\quad + (1-2\alpha) \beta r_{t-1} - Q_{1t-1} & (\text{expand and simplify})
\end{aligned}$$

resulting in

$$\frac{\partial^2 Q_{1t}}{\partial x_2^2} = (1-\alpha) \frac{\partial^2 Q_{1t-1}}{\partial x_2^2} - 2(\alpha(1-\alpha)) \frac{\partial Q_{1t-1}}{\partial x_2} + (1-2\alpha) \beta r_{t-1} - Q_{1t-1} \quad (D.22)$$

Finally, we expand equation (C.21) using equation (C.22) to obtain the second-order direct partial derivative of LL_{A_t} with respect to x_2 .

Solve for $\frac{\partial^2 LL_{A_t}}{\partial x_2 \partial x_1}$:

$$\begin{aligned} \frac{\partial^2 LL_{A_t}}{\partial x_2 \partial x_1} &= \frac{\partial^2 Q_{1_t}}{\partial x_2 \partial x_1} - \left[e^{LL_{A_t}} \frac{\partial^2 Q_{1_t}}{\partial x_2 \partial x_1} + \frac{\partial Q_{1_t}}{\partial x_2} \left(\frac{\partial LL_{A_t}}{\partial x_1} e^{LL_{A_t}} \right) \right] \\ &\quad - \left[(1 - e^{LL_{A_t}}) \frac{\partial^2 Q_{2_t}}{\partial x_2 \partial x_1} + \frac{\partial Q_{2_t}}{\partial x_2} \left(-\frac{\partial LL_{A_t}}{\partial x_1} e^{LL_{A_t}} \right) \right] \quad (\text{cross partial derivative of (C.15) of } x_1 \text{ w.r.t } x_2) \end{aligned}$$

resulting in

$$\frac{\partial^2 LL_{A_t}}{\partial x_2 \partial x_1} = \frac{\partial^2 Q_{1_t}}{\partial x_2 \partial x_1} - \left[e^{LL_{A_t}} \frac{\partial^2 Q_{1_t}}{\partial x_2 \partial x_1} + (1 - e^{LL_{A_t}}) \left(\frac{\partial^2 Q_{2_t}}{\partial x_2 \partial x_1} \right) \right] - \frac{\partial LL_{A_t}}{\partial x_1} e^{LL_{A_t}} \left(\frac{\partial Q_{1_t}}{\partial x_2} - \frac{\partial Q_{2_t}}{\partial x_2} \right) \quad (\text{D.23})$$

To solve for $\frac{\partial^2 Q_{1_t}}{\partial x_2 \partial x_1}$ in equation (C.23), we will refer to equation (C.13) and differentiate with respect to x_2 :

Solve for $\frac{\partial^2 Q_{1_t}}{\partial x_2 \partial x_1}$:

$$\begin{aligned} \frac{\partial Q_{1_t}}{\partial x_2} &= (1 - \alpha) \frac{\partial Q_{1_{t-1}}}{\partial x_2} + (\beta r_{t-1} - Q_{1_{t-1}}) \frac{\partial \alpha}{\partial x_2} \quad (\text{C.13}) \\ \frac{\partial^2 Q_{1_t}}{\partial x_2 \partial x_1} &= (1 - \alpha) \frac{\partial^2 Q_{1_{t-1}}}{\partial x_2 \partial x_1} + (\beta r_{t-1} - Q_{1_{t-1}}) \frac{\partial^2 \alpha}{\partial x_2 \partial x_1} \\ &\quad + \left(\frac{\partial \beta}{\partial x_1} r_{t-1} - \frac{\partial Q_{1_{t-1}}}{\partial x_1} \right) \frac{\partial \alpha}{\partial x_2} \quad (\text{cross partial derivative of } x_1 \text{ w.r.t } x_2) \\ &= (1 - \alpha) \frac{\partial^2 Q_{1_{t-1}}}{\partial x_2 \partial x_1} + (\alpha(1 - \alpha)) \left[\beta r_{t-1} - \frac{\partial Q_{1_{t-1}}}{\partial x_1} \right] \quad (\text{expand and simplify}) \end{aligned}$$

resulting in

$$\frac{\partial^2 Q_{1_t}}{\partial x_2 \partial x_1} = (1 - \alpha) \frac{\partial^2 Q_{1_{t-1}}}{\partial x_2 \partial x_1} + (\alpha(1 - \alpha)) \left[\beta r_{t-1} - \frac{\partial Q_{1_{t-1}}}{\partial x_1} \right] \quad (\text{D.24})$$

Finally, we expand equation (C.23) using equation (C.24) to obtain the second-order cross partial derivative of LL_{A_t} of x_1 with respect to x_2 .