

Transforming complex to real:

$$\bar{J}(\psi, u) = \frac{1}{2} \langle \psi, \bar{Q}\psi \rangle + \frac{1}{2} \langle u, Ru \rangle$$

$$\text{s.t. } \dot{\psi} = -i(H_0 + uV)\psi; \quad \psi(0) = \psi_0$$

$$\text{Let } \psi = \psi_x + i\psi_y; \quad \bar{J}(\psi_x, \psi_y, u) = \bar{J}(\psi = \psi_x + i\psi_y, u)$$

$$\bar{J}(\psi_x, \psi_y, u) = \frac{1}{2} \langle \psi_x + i\psi_y, Q(\psi_x + i\psi_y) \rangle + \frac{1}{2} \langle u, Ru \rangle$$

$$= \frac{1}{2} \left\langle \begin{bmatrix} \psi_x \\ \psi_y \end{bmatrix}, Q \begin{bmatrix} \psi_x \\ \psi_y \end{bmatrix} \right\rangle + \frac{1}{2} \langle u, Ru \rangle \quad \left(Q = \begin{bmatrix} \bar{Q} & 0 \\ 0 & \bar{Q} \end{bmatrix} \right)$$

$$\frac{d}{dt}(\psi_x + i\psi_y) = -i(H_0 + uV)(\psi_x + i\psi_y)$$

$$\Rightarrow \dot{\psi}_x = (H_0 + uV)\psi_y$$

$$\dot{\psi}_y = -(H_0 + uV)\psi_x$$

$$\text{Let } x = \begin{bmatrix} \psi_x \\ \psi_y \end{bmatrix} \quad \text{Hence the real optimal control problem is:}$$

$$\bar{J}(x, u) = \frac{1}{2} \langle x, Qx \rangle + \frac{1}{2} \langle u, Ru \rangle$$

$$\text{s.t. } \dot{x} = (A + Bu)x \quad x(0) = x_0$$

$$\text{with } A := \begin{bmatrix} 0 & H_0 \\ -H_0 & 0 \end{bmatrix}; \quad B := \begin{bmatrix} 0 & V \\ -V & 0 \end{bmatrix}; \quad x_0 = \begin{bmatrix} \text{real}(\psi_0) \\ \text{imag}(\psi_0) \end{bmatrix}$$

$$x := \begin{bmatrix} \text{real}(\psi) \\ \text{imag}(\psi) \end{bmatrix} \quad Q := \begin{bmatrix} \bar{Q} & 0 \\ 0 & \bar{Q} \end{bmatrix}$$

$$\text{Consider } \bar{J}(x, u) = \int_0^T \left\{ \frac{1}{2} x^T(\tau) Q x(\tau) + \frac{R}{2} u^2(\tau) \right\} d\tau$$

$$\begin{cases} \dot{x}(t) = (A + u(t)B)x(t) \\ x(0) = x_0 \end{cases}$$

Gradient Descent:

$$\text{Let } H(x(t), u(t), \lambda(t)) := \frac{1}{2} x^T(t) Q x(t) + \frac{R}{2} u^2(t) + \lambda^T(t) (A + u(t)B)x(t)$$

$$\Rightarrow \dot{\lambda}(t) = - \frac{\partial H}{\partial x}(x(t), u(t), \lambda(t)) = -Qx(t) - (A^T + u(t)B^T)\lambda(t)$$

$$\frac{\partial H(x(t), u(t), \lambda(t))}{\partial u} = Ru(t) + x(t)^T B^T \lambda(t)$$

Algorithm: 1. Guess $u_0(t)$; $k=0$

2. Iterate

$$\begin{aligned} 2a. & \text{ Solve for } x_k: \quad \dot{x}_k = (A + u_k B)x_k; \quad x_k(0) = x_0 \\ 2b. & \text{ Solve for } \lambda_k: \quad \dot{\lambda}_k = -(A^T + u_k B^T)\lambda_k - Qx_k; \quad \lambda_k(T) = 0 \end{aligned}$$

2.c. Calculate $\frac{\partial H_x}{\partial u} = R u_x + x_k' B' \lambda$

3. Update: $u_{k+1}(t) = u_k(t) - \alpha_k (R u_k(t) + \lambda^T u_k(t) B^T x_k(t))$

4. If $\left\| \frac{\partial H}{\partial u} \right\| < \text{ETOL} \Rightarrow \text{stop}$; otherwise $k = k+1$ and go to step 2

Modified Gradient Descent:

Let $\tilde{x} := Q^{1/2}x$; $\tilde{u} := R^{1/2}u$ and $\tilde{J}(\tilde{x}, \tilde{u}) := J(x, u)$

$$(H_0 + H_1 u_1 + H_2 u_2)^x$$

$$\Rightarrow \tilde{J}(\tilde{x}, \tilde{u}) = \frac{1}{2} \langle \tilde{x}, \tilde{x} \rangle + \frac{1}{2} \langle \tilde{u}, \tilde{u} \rangle$$

$$\begin{cases} \ddot{\tilde{x}} = Q^{\frac{1}{2}}(A + BR^{-\frac{1}{2}}\tilde{u})Q^{\frac{1}{2}}\tilde{x} := (\tilde{A} + \tilde{B}u)\tilde{x} \\ \tilde{x}(0) = Q^{\frac{1}{2}}x_0 =: \tilde{x}_0 \end{cases}$$

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Let $z = \begin{bmatrix} x \\ u \end{bmatrix}$ $G(z): \mathbb{L}_2^{n+m}([0, T]) \longrightarrow \mathbb{L}_2^n([0, T]) \times \mathbb{R}^r$

$\begin{bmatrix} x \\ u \end{bmatrix} \longmapsto \left[\begin{bmatrix} \frac{d}{dt} - (A + Bu) \end{bmatrix} x \right]$

$S_0 x := x(0)$ $S_0 x - x_0$

$$\Rightarrow \frac{\partial G}{\partial z}(z_k): \mathbb{L}_2^{nm}([0, T]) \longrightarrow \mathbb{L}_2^n([0, T]) \times \mathbb{R}^r$$

$$\begin{bmatrix} \delta x \\ \delta u \end{bmatrix} \longmapsto \begin{bmatrix} \frac{d}{dt} - (A + B u_k) & -B x_k \\ s_0 & 0 \end{bmatrix} \begin{bmatrix} \delta x \\ \delta u \end{bmatrix}$$

$$\Rightarrow \frac{\partial G^*(z_k)}{\partial z} : \mathbb{D} \left(\frac{\partial G^*(z_k)}{\partial z} \right) \xrightarrow{\quad} \mathbb{L}_2^{nn}([0, T])$$

$$\begin{bmatrix} \lambda \\ \mu \end{bmatrix} \mapsto - \begin{bmatrix} \frac{d}{dt} + (A + B u_k)^T \\ (B x_k)^T \end{bmatrix} \begin{bmatrix} \lambda \\ \mu \end{bmatrix}$$

with $\mathbb{D} \left(\frac{\partial G^x}{\partial z}(z_k) \right) := \left\{ \begin{bmatrix} \lambda \\ \mu \end{bmatrix} \in \mathbb{H}_2^n \times \mathbb{R}^n; \lambda(T) = 0 \text{ and } \mu = \lambda(0) \right\}$

$$\Rightarrow \left[\frac{\partial G}{\partial z} \right] \cdot \left[\frac{\partial G^*}{\partial z} \right] \begin{bmatrix} \lambda \\ \mu \end{bmatrix} = - \begin{bmatrix} \frac{d}{dt} - (A + B u_k) & - B x_k \\ 0 & (B x_k)^T \end{bmatrix} \begin{bmatrix} \lambda \\ \mu \end{bmatrix}$$

$$= \begin{bmatrix} \left[\frac{d}{dt} - (A + Bu_k) \right] \cdot \left[\frac{d}{dt} + (A + Bu_k)^T \right] + (Bx_k)(Bx_k)^T & 0 \\ -S_0 \cdot \left[\frac{d}{dt} + (A + Bu_k)^T \right] & 0 \end{bmatrix} \begin{bmatrix} \lambda \\ \mu \end{bmatrix}$$

$$= \left[-\frac{d^2}{dt^2} - (A + B u_k)^T \frac{d}{dt} - \left(B \frac{d u_k}{dt} \right)^T + (A + B u_k) \frac{d}{dt} + (A + B u_k)(A + B u_k)^T + (B x_k)(B x_k)^T \right] \lambda$$

$$= \left[\frac{d^2 \lambda}{dt^2} + [A - A^T + u_k (B - B^T)] \frac{d\lambda}{dt} + [(A + Bu_k)(A + Bu_k)^T + (Bx_k)(Bx_k)^T - \frac{du_k}{dt} B^T] \lambda \right. \\ \left. - \frac{d}{dt} \lambda(0) - [A^T + u_k(0) B^T] \lambda(0) \right]$$

The update rule is: $u_{k+1} = u_k - \alpha_k [0 \ I]^T \nabla \left(\frac{\partial \mathcal{L}(z_k)}{\partial z} \right) (z_k)$

$$2G_{12}^* \nabla_{\bar{z}_k}^T (2G_{\bar{z}_k}) (z_k)$$

The update rule is: $u_{k+1} = u_k - \alpha_k [0 \ I]^T \nabla \left(\frac{\partial G}{\partial z} \right) (z_k)$

$$\text{But } \Pi_{\nabla \left(\frac{\partial G}{\partial z} \right) (z_k)} (z_k) = z_k - \frac{\partial G^*}{\partial z} (z_k) \cdot \underbrace{\left[\frac{\partial G}{\partial z} (z_k) \cdot \frac{\partial G^*}{\partial z} (z_k) \right]^{-1}}_{\begin{bmatrix} \lambda_k \\ \mu_k \end{bmatrix}} \left(\frac{\partial G}{\partial z} \right) (z_k)$$

$$\Rightarrow \left[\frac{\partial G}{\partial z} (z_k) \cdot \frac{\partial G^*}{\partial z} (z_k) \right]^{-1} \left(\frac{\partial G}{\partial z} \right) (z_k) = \begin{bmatrix} \lambda_k \\ \mu_k \end{bmatrix}$$

$$\Rightarrow \left[\frac{\partial G}{\partial z} (z_k) \cdot \frac{\partial G^*}{\partial z} (z_k) \right] \begin{bmatrix} \lambda_k \\ \mu_k \end{bmatrix} = \left(\frac{\partial G}{\partial z} \right) (z_k)$$

$$\begin{aligned} \Rightarrow -\frac{d^2}{dt^2} \lambda_k + [A - A^T + u_k (B - B^T)] \frac{d}{dt} \lambda_k + [(A + Bu_k)(A + Bu_k)^T + (Bx_k)(Bx_k)^T - \frac{du_k}{dt} B^T] \lambda_k \\ = \left(\frac{d}{dt} - (A + Bu_k) \right) x_k - Bx_k u_k \\ = (A + Bu_k) x_k - (A + Bu_k) x_k - Bx_k u_k \\ = -Bx_k u_k \end{aligned}$$

$$\text{s.t. } -\frac{d}{dt} \lambda_k(0) - (A + Bu_k(0))^T \lambda_k(0) = x_k(0)$$

Therefore:

$$\frac{d}{dt} \begin{bmatrix} \lambda_k \\ \dot{\lambda}_k \end{bmatrix} = \begin{bmatrix} 0 & I \\ (A + Bu_k)(A + Bu_k)^T + (Bx_k)(Bx_k)^T - \frac{du_k}{dt} B^T & A - A^T + u_k (B - B^T) \end{bmatrix} \begin{bmatrix} \lambda_k \\ \dot{\lambda}_k \end{bmatrix} + \begin{bmatrix} 0 \\ Bx_k u_k \end{bmatrix}$$

$$\text{s.t. } \frac{d}{dt} \lambda_k(0) + (A + Bu_k(0))^T \lambda_k(0) = -x_k(0)$$

$$\lambda_k(T) = 0$$

$$\Rightarrow u_{k+1} = u_k - \alpha_k \left(u_k - [0 \ I]^T \left(\frac{\partial G^*}{\partial z} \right) \left(\begin{bmatrix} \lambda \\ \dot{\lambda} \end{bmatrix} \right) \right)$$

$$= u_k - \alpha_k (u_k + \lambda_k^T Bx_k)$$

Algorithm:

1. Guess $\tilde{u}_0(t)$; $k=0$

2. $\tilde{A} := Q^{1/2} A Q^{1/2}$; $\tilde{B} := Q^{1/2} B R^{-1/2} Q^{1/2}$; $\tilde{x}_0 = Q^{1/2} x$

3. Iterate:

3.a Solve for \tilde{x}_k : $\dot{\tilde{x}}_k = (\tilde{A} + \tilde{B} \tilde{u}_k) \tilde{x}_k$; $\tilde{x}_k(0) = \tilde{x}_0$

3.b Solve for λ_k :

$$\frac{d}{dt} \begin{bmatrix} \lambda_k \\ \dot{\lambda}_k \end{bmatrix} = \begin{bmatrix} 0 & I \\ (\tilde{A} + \tilde{B} \tilde{u}_k)(\tilde{A} + \tilde{B} \tilde{u}_k)^T + (\tilde{B} \tilde{x}_k)(\tilde{B} \tilde{x}_k)^T - \frac{d\tilde{u}_k}{dt} \tilde{B}^T & \tilde{A} - \tilde{A}^T + \tilde{u}_k (\tilde{B} - \tilde{B}^T) \end{bmatrix} \begin{bmatrix} \lambda_k \\ \dot{\lambda}_k \end{bmatrix} + \begin{bmatrix} 0 \\ \tilde{B} \tilde{x}_k \tilde{u}_k \end{bmatrix}$$

$$\text{s.t. } \frac{d}{dt} \lambda_k(0) + (\tilde{A} + \tilde{B} \tilde{u}_k(0))^T \lambda_k(0) = -\tilde{x}_k(0)$$

$$\lambda_k(T) = 0$$

3.c Calculate $\frac{\partial H_k}{\partial u} = \tilde{u}_k + \tilde{x}_k^T \tilde{B}^T \lambda_k$

4. Update: $\tilde{u}_{k+1}(t) = \tilde{u}_k(t) - \alpha_k [\tilde{u}_k(t) + \tilde{x}_k^T(t) \tilde{B}^T \lambda_k(t)]$

5. If $\left\| \frac{\partial H_k}{\partial u} \right\| < \epsilon \Rightarrow$ go to step 6, otherwise: $k = k+1$ and go to step 3

$$\dots \dots \dots R^{-1/2} \tilde{u}(t)$$

6. $x(t) = Q^{-1/2} \tilde{x}(t)$ and $u(t) = R^{-1/2} \tilde{u}(t)$

How to solve for λ_k ?

Drop the "k" and the "~" and let $\dot{\lambda}(t) = P(t)\lambda(t) + \omega(t)$

$$\Rightarrow \ddot{\lambda}(t) = \dot{P}(t)\lambda(t) + P(t)[P(t)\lambda(t) + \omega(t)] + \dot{\omega}(t)$$

$$\Rightarrow [(A + Bu)(A + Bu)^T + (Bx)(Bx)^T - \dot{u}B^T]\lambda + [A - A^T + u(B - B^T)][P\lambda + \omega] + Bx u$$

$$= \dot{P}\lambda + P^2\lambda + P\omega + \dot{\omega}$$

$$\Rightarrow (A + Bu)(A + Bu)^T + (Bx)(Bx)^T - \dot{u}B^T + [A - A^T + u(B - B^T)]P - P^2 = \dot{P}$$

and $[A - A^T + u(B - B^T) - P]\omega + Bx u = \dot{\omega}$

$$\dot{\lambda}(0) = P(0)\lambda(0) + \omega(0) \Rightarrow \begin{cases} \omega(0) = -x(0) \\ P(0) = -(A + Bu(0))^T \end{cases}$$

Therefore, to solve for λ_k :

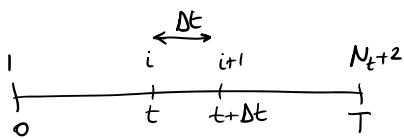
1. $\dot{P}_k = [\tilde{A} - \tilde{A}^T + \tilde{u}_k(\tilde{B} - \tilde{B}^T)]P_k - P_k^2 + (\tilde{A} + \tilde{B}\tilde{u}_k)(\tilde{A} + \tilde{B}\tilde{u}_k)^T + (\tilde{B}\tilde{x}_k)(\tilde{B}\tilde{x}_k)^T - \dot{\tilde{u}}_k\tilde{B}^T$
 $P_k(0) = -(\tilde{A} + \tilde{B}\tilde{u}_k(0))^T$
2. $\dot{w}_k = [\tilde{A} - \tilde{A}^T + \tilde{u}_k(\tilde{B} - \tilde{B}^T) - P_k]\omega + \tilde{B}\tilde{x}_k\tilde{u}_k$
 $w_k(0) = -\tilde{x}_k(0)$
3. $\dot{\lambda}_k = P_k\lambda_k + w_k$
 $\lambda_k(T) = 0$

Another Method:

$$\ddot{\lambda}(t) + F(t)\dot{\lambda}(t) + W(t)\lambda(t) = V(t)$$

$$M_0\dot{\lambda}(0) + N_0\lambda(0) = m_0$$

$$M_T\dot{\lambda}(T) + N_T\lambda(T) = m_T$$



$$t_i := (i-1)\Delta t \quad \Delta t := \frac{T}{N_t+1}$$

$$i = 1, 2, \dots, N_t+2$$

$$\lambda_i := \lambda(t_i) \quad ; \quad F_i := F(t_i) \quad ; \quad W_i := W(t_i) \quad ; \quad V_i := V(t_i)$$

$$\frac{\lambda_{i+1} - 2\lambda_i + \lambda_{i-1}}{\Delta t^2} + F_i \frac{\lambda_{i+1} - \lambda_{i-1}}{2\Delta t} + W_i\lambda_i = V_i \quad i = 2, 3, \dots, N_t+1$$

$$\Rightarrow \left[\left(\frac{1}{\Delta t^2} - \frac{F_i}{2\Delta t} \right) \lambda_{i-1} + \left(W_i - \frac{2F_i}{\Delta t^2} \right) \lambda_i + \left(\frac{1}{\Delta t^2} + \frac{F_i}{2\Delta t} \right) \lambda_{i+1} = V_i \quad ; i = 2, \dots, N_t+1 \right]$$

$$M_0 \frac{\lambda_2 - \lambda_0}{2\Delta t} + N_0\lambda_1 = m_0 \Rightarrow \lambda_0 = \lambda_2 + 2\Delta t M_0^{-1}(N_0\lambda_1 - m_0)$$

$$M_T \frac{\lambda_{N_t+3} - \lambda_{N_t+1}}{2\Delta t} + N_T\lambda_{N_t+2} = m_T$$

$$\Rightarrow \lambda_{N_t+1} - \lambda_{N_t+3} + 2\Delta t M_T^{-1}(m_T - N_T\lambda_{N_t+2})$$

$$M_T \frac{\lambda_{N_t+3} - \lambda_{N_t+1}}{2\Delta t} + N_T \lambda_{N_t+2} = m_T \Rightarrow \lambda_{N_t+3} = \lambda_{N_t+1} + 2\Delta t M_T^{-1} (m_T - N_T \lambda_{N_t+2})$$

$$\Rightarrow \left(W_1 - \frac{2I}{\Delta t^2} \right) \lambda_1 + \left(\frac{I}{\Delta t^2} + \frac{F_1}{2\Delta t} \right) \lambda_2 + \left(\frac{I}{\Delta t^2} - \frac{F_1}{2\Delta t} \right) \left[\lambda_2 + 2\Delta t M_0^{-1} N_0 \lambda_1 - 2\Delta t M_0^{-1} m_0 \right] = V_1$$

$$\Rightarrow \left[W_1 - \frac{2I}{\Delta t^2} + \left(\frac{I}{\Delta t^2} - \frac{F_1}{2\Delta t} \right) 2\Delta t M_0^{-1} N_0 \right] \lambda_1 + \left[\frac{2I}{\Delta t^2} \right] \lambda_2 = V_1 + 2\Delta t \left(\frac{I}{\Delta t^2} - \frac{F_1}{2\Delta t} \right) M_0^{-1} m_0$$

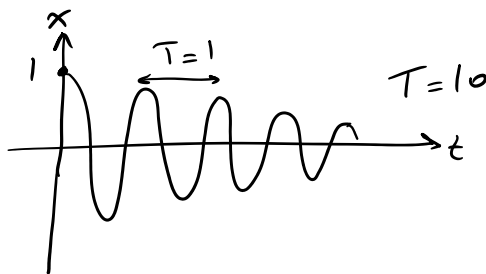
$$\left(W_{N_t+2} - \frac{2I}{\Delta t^2} \right) \lambda_{N_t+2} + \left(\frac{I}{\Delta t^2} - \frac{F_{N_t+2}}{2\Delta t} \right) \lambda_{N_t+1} + \left(\frac{I}{\Delta t^2} + \frac{F_{N_t+2}}{2\Delta t} \right) \left[\lambda_{N_t+1} + 2\Delta t M_T^{-1} (m_T - N_T \lambda_{N_t+2}) \right] = V_{N_t+2}$$

$$\Rightarrow \left[\frac{2I}{\Delta t^2} \right] \lambda_{N_t+1} + \left[W_{N_t+2} - \frac{2I}{\Delta t^2} - \left(\frac{I}{\Delta t^2} + \frac{F_{N_t+2}}{2\Delta t} \right) 2\Delta t M_T^{-1} N_T \right] \lambda_{N_t+2} = V_{N_t+2} - 2\Delta t \left(\frac{I}{\Delta t^2} + \frac{F_{N_t+2}}{2\Delta t} \right) M_T^{-1} m_T$$

$$\left(\frac{I}{\Delta t^2} - \frac{F_i}{2\Delta t} \right) \lambda_{i-1} + \left(W_i - \frac{2I}{\Delta t^2} \right) \lambda_i + \left(\frac{I}{\Delta t^2} + \frac{F_i}{2\Delta t} \right) \lambda_{i+1} = V_i \quad i=2, \dots, N_t+1$$

$$\begin{bmatrix} T_1 & \frac{2I}{\Delta t^2} & & & & & \\ \frac{I}{\Delta t^2} - \frac{F_2}{2\Delta t} & W_2 - \frac{2I}{\Delta t^2} & \frac{I}{\Delta t^2} + \frac{F_2}{2\Delta t} & & & & \\ & \frac{I}{\Delta t^2} - \frac{F_3}{2\Delta t} & W_3 - \frac{2I}{\Delta t^2} & \frac{I}{\Delta t^2} + \frac{F_3}{2\Delta t} & & & \\ & & & & \ddots & & \\ & & & & & \frac{I}{\Delta t^2} - \frac{F_{N_t+1}}{2\Delta t} & W_{N_t+1} - \frac{2I}{\Delta t^2} & \frac{I}{\Delta t^2} + \frac{F_{N_t+1}}{2\Delta t} \\ & & & & & & \frac{2I}{\Delta t^2} & T_T \\ & & & & & & & \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \vdots \\ \lambda_{N_t+1} \\ \lambda_{N_t+2} \end{bmatrix} = \begin{bmatrix} V_1 + b_1 \\ V_2 \\ V_3 \\ \vdots \\ V_{N_t+1} \\ V_{N_t+2} - b_T \end{bmatrix}$$

$$x(t) = e^{-t} \cos(2\pi t)$$



$$\dot{x}(t) = -e^{-t} \cos(2\pi t) - e^{-t} \cdot 2\pi \sin(2\pi t) = -x(t) - 2\pi e^{-t} \sin(2\pi t)$$

$$\ddot{x}(t) = -\dot{x}(t) - 2\pi(-1)e^{-t} \sin(2\pi t) - 2\pi e^{-t} \cdot 2\pi \cos(2\pi t)$$

$$= -\dot{x}(t) + 2\pi e^{-t} \sin(2\pi t) - 4\pi^2 x(t)$$

$$\Rightarrow \ddot{x}(t) + \dot{x}(t) + 4\pi^2 x(t) = 2\pi e^{-t} \sin(2\pi t)$$

$$N_0 = 1 \quad m_0 = 1$$

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$$\Rightarrow \ddot{x}(t) + \dot{x}(t) + 4\pi^2 x(t) = 2\pi e^{-t} \sin(2\pi t)$$

$$\boxed{\begin{aligned} x(0) &= 1 \\ x(T) &= e^{-1} \end{aligned}}$$

$$\dot{x}(T) = -e^{-1}$$

$$M_i \ddot{x}(i) + N_i \dot{x}(i) = m_i$$

$$\begin{aligned} M_0 &= 0 & N_0 &= 1 & m_0 &= 0 \\ M_T &= 1 & N_T &= 0 & m_T &= 0 \end{aligned}$$