

# Adjoint Equation

## General problem

Looking at an optimal control problem

$$\min_{y,u} J(y,u) \text{ subject to } E(y,u) = 0$$

Where  $u \in L^2(\Omega)$  and  $y \in H^1(\Omega)$ , with  $\Omega = (0, T)$ . I have chosen these spaces because they are Hilbert spaces, however I will for the most part ignore them.  $J$  is a functional on  $L^2(\Omega) \times H^1(\Omega)$  and  $E$  is an operator on  $H^1(\Omega)$ . Both  $J$  and  $E$  need certain properties described elsewhere.

Differentiating  $J$  is required for solving the problem. To do this we reduce  $J$  to  $\hat{J}(u) = J(y(u), u)$  and compute its gradient in direction  $s \in L^2(\Omega)$ . Will use the notation:  $\langle \hat{J}'(u), s \rangle$  for the gradient.

$$\begin{aligned} \langle \hat{J}'(u), s \rangle &= \left\langle \frac{\partial J(y(u), u)}{\partial u}, s \right\rangle \\ &= \left\langle \frac{\partial y(u)}{\partial u}^* J_y(y(u), u), s \right\rangle + \langle J_u(y(u), u), s \rangle \\ &= \langle y'(u)^* J_y(u), s \rangle + \langle J_u(u), s \rangle \end{aligned}$$

Here  $\langle \cdot, \cdot \rangle$  is the  $L^2$  inner product. The difficult term in the expression above is  $y'(u)^*$ , so lets first differentiate  $E(y(u), u) = 0$  with respect to  $u$ , and try to find an expression for  $y'(u)^*$ :

$$\begin{aligned} \frac{\partial}{\partial u} E(y(u), u) = 0 &\Rightarrow E_y(y(u), u) y'(u) = -E_u(y(u), u) \\ &\Rightarrow y'(u) = -E_y(y(u), u)^{-1} E_u(y(u), u) \\ &\Rightarrow y'(u)^* = -E_u(y(u), u)^* E_y(y(u), u)^{-*} \end{aligned}$$

By inserting our new expression for  $y'(u)^*$  into  $y'(u)^* J_y(u)$ , we get:

$$\begin{aligned} y'(u)^* J_y(u) &= -E_u(y(u), u)^* E_y(y(u), u)^{-*} J_y(u) \\ &= -E_u(y(u), u) \lambda \end{aligned}$$

$\lambda$  is here the solution of the adjoint equation

$$E_y(y(u), u)^* \lambda = J_y(u)$$

If we can solve this equation for  $\lambda$ , the gradient of  $\hat{J}$  will be given by the following formula:

$$\langle \hat{J}'(u), s \rangle = \langle -E_u(y(u), u) \lambda, s \rangle + \langle J_u(u), s \rangle \quad (1)$$

### Specific problem and differentiation of the operators

We now look at an example of the above problem, and try to derive the adjoint equation and the gradient. Let  $J$  be defined as:

$$J(y, u) = \frac{1}{2} \int_0^T u^2 dt + \frac{1}{2} (y(T) - y^T)^2 \quad (2)$$

and let our ODE constraint be:

$$\begin{cases} E(y, u) = y' - \alpha y - u \\ y(0) = y_0 \end{cases} \quad (3)$$

Before we derive the adjoint equation, lets find  $E_u$ ,  $E_y$ ,  $\langle J_u(u), s \rangle$  and  $J_y$  with respect to our  $E$  and  $J$ .

$$E_u(y(u), u) = -1$$

$$E_y(y(u), u) = \frac{\partial}{\partial t} - \alpha + \delta_0, \text{ where } \delta_0 \text{ is evaluation at } 0$$

$$\langle J_u(u), s \rangle = \int_0^T u(t)s(t)dt$$

Lets be more thorough with  $J_y$ , which is the right hand side in the adjoint equation.

$$\begin{aligned} J_y(y(u), u) &= \frac{\partial}{\partial y} \left( \frac{1}{2} \int_0^T u^2 dt + \frac{1}{2} (y(T) - y^T)^2 \right) \\ &= \frac{\partial}{\partial y} \frac{1}{2} (y(T) - y^T)^2 \\ &= \frac{\partial}{\partial y} \frac{1}{2} \left( \int_0^T \delta_T (y - y^T) dt \right)^2 \\ &= \delta_T \int_0^T \delta_T (y(t) - y^T) dt \\ &= \delta_T (y(T) - y^T) = L \end{aligned}$$

Here I have use some dirac-delta tricks, that may not be valid, but the result is probably correct. By  $\delta_T(y(T) - y^T)$ , I mean evaluation at time  $T$ , of the constant function  $y(T) - y^T$ .

### Deriving the adjoint equation

We have  $E_y(y(u), u) = \frac{\partial}{\partial t} - \alpha + \delta_0$ , but for the adjoint equation we need to find  $E_y^*$ . To derive the adjoint of  $E_y$ , we will apply it to a function  $v$  and then take the  $L^2$  inner product with another function  $w$ . The next step is then to try to "move" the operator  $E_y$  from  $v$  to  $w$ . As becomes clear below,

partial integration is the main trick to achieve this:

$$\begin{aligned}
\langle E_y v, w \rangle &= \int_0^T (v'(t) - \alpha v(t) + \delta_0 v(t)) w(t) dt \\
&= \int_0^T v'(t) w(t) dt - \alpha \int_0^T v(t) w(t) dt + v(0) w(0) \\
&= - \int_0^T v(t) w'(t) dt + v(t) w(t) \Big|_0^T - \alpha \langle v, w \rangle + v(0) w(0) \\
&= - \int_0^T v(t) w'(t) dt - \alpha \langle v, w \rangle + v(T) w(T) \\
&= \langle v, Pw \rangle
\end{aligned}$$

Where  $P = -\frac{\partial}{\partial t} - \alpha + \delta_T$ . This means that  $E_y^* = P$ , and we now have the left hand side in the adjoint equation. The right hand side is  $J_y(y(u), u) = L$ , which we have already found. If we write the adjoint equation on variational form it will look like this:  $\langle P\lambda, w \rangle = \langle L, w \rangle$ . To get back to standard ODE form, we can do some manipulation:

$$\begin{aligned}
\langle -\lambda' - \alpha\lambda + \delta_T \lambda, w \rangle &= \langle \delta_T(y(T) - y^T), w \rangle \\
\langle -\lambda' - \alpha\lambda, w \rangle &= \langle \delta_T(y(T) - y^T - \lambda), w \rangle
\end{aligned}$$

The right hand side is point evaluation at  $t = T$ , while the left hand side is an expression for all  $t$ . This finally gives us our adjoint equation:

$$\begin{cases} -\lambda'(t) - \alpha\lambda(t) = 0 \\ \lambda(T) = y(T) - y^T \end{cases} \quad (4)$$

This is a simple and easily solvable ODE.

### Expression for the gradient

We now have all the ingredients for finding an expression for the gradient of  $\hat{J}$ . If we remember that  $\langle \hat{J}'(u), s \rangle = \langle y'(u)^* J_y(u), s \rangle + \langle J_u(u), s \rangle$ , and all the different expressions for all the terms we calculated, we find:

$$\begin{aligned}
\langle \hat{J}'(u), s \rangle &= \langle y'(u)^* J_y(u), s \rangle + \langle J_u(u), s \rangle \\
&= \langle -E_u^* \lambda, s \rangle + \langle J_u(u), s \rangle \\
&= \langle -(-1)^* \lambda, s \rangle + \langle u, s \rangle \\
&= \langle \lambda + u, s \rangle \\
&= \int_0^T (\lambda(t) + u(t)) s(t) dt
\end{aligned}$$

Note that the adjoint of a constant is just the constant itself.

### Simple example

Let  $T = y_T = y_0 = \alpha = 1$  and assume that we want to find the gradient of  $\hat{J}$  at  $u(t) = 0$ . We then have:

$$J(y, u) = \frac{1}{2} \int_0^1 u^2 dt + \frac{1}{2} (y(T) - 1)^2 \quad (5)$$

and

$$\begin{cases} E(y, u) = y' - y + u \\ y(0) = 1 \end{cases} \quad (6)$$

Since  $u = 0$ , we easily find  $y(t) = e^t$ . This gives us the adjoint equation:

$$\begin{cases} -\lambda'(t) - \lambda(t) = 0 \\ \lambda(T) = e - 1 \end{cases} \quad (7)$$

This is again a simple equation which yields  $\lambda(t) = (e - 1)e^{1-t}$ . The gradient of  $\hat{J}$  is then:

$$\langle \hat{J}'(u), s \rangle = \int_0^1 (e - 1)e^{1-t} s(t) dt$$

### Discretization

Let us discretize our interval  $[0, T]$  using  $N + 1$  points where

$$x_n = n\Delta t, \quad i = 0, \dots, N \quad \text{and} \\ \Delta t = \frac{T}{N}$$

We also let  $y^n = y(x^n)$  and  $u^n = u(x^n)$ . The integrals in our functional and its gradient we evaluate using the trapezoidal rule, and we discretize our ODE  $E(y, u) = 0$  and the adjoint equation using the Backward Euler scheme. For  $E(y, u) = 0$  we get :

$$\begin{aligned} \frac{y^n - y^{n-1}}{\Delta t} &= \alpha y^n + u^n \\ (1 - \alpha\Delta t)y^n &= y^{n-1} + \Delta t u^n \\ y^n &= \frac{y^{n-1} + \Delta t u^n}{1 - \alpha\Delta t} \end{aligned}$$

Here the initial condition  $y^0 = y_0$  is known. For the adjoint equation the initial condition is  $\lambda^N = y^N - y^T$ , and the Backward Euler scheme gives us:

$$\begin{aligned} -\frac{\lambda^n - \lambda^{n-1}}{\Delta t} - \alpha\lambda^n &= 0 \\ \lambda^{n-1} - \lambda^n &= \Delta t \alpha \lambda^n \\ \lambda^{n-1} &= (1 + \Delta t \alpha) \lambda^n \end{aligned}$$

### The discrete gradient

So we now have a way of solving our ODEs numerically. In the continuous case the gradient was  $\int_0^T (\lambda(t) + u(t))s(t)dt$ , however in the discrete case,  $\hat{J}$  is a function dependent on the  $N + 1$  values of  $u$ . This would suggest that the gradient of  $\hat{J}$  should be a vector of size  $N + 1$ . The thing that makes the most sense to me is to insert the unit vectors of  $\mathbb{R}^{N+1}$  into our continuous gradient, and then evaluate the integral using the trapezoidal rule. Based on experiments using finite difference for calculating  $\hat{J}$ , this approach works for  $n \neq 0$  and  $n \neq N$ . Without more explanation I will assert that our discrete gradient  $\hat{J}'_{\Delta t}(u)$  looks like this:

$$\begin{aligned}\hat{J}'_{\Delta t}(u)^n &= \Delta t(u^n + \lambda^n) \text{ when } n = 1, \dots, N - 1 \\ \hat{J}'_{\Delta t}(u)^0 &= \Delta t \frac{1}{2} u^0 \\ \hat{J}'_{\Delta t}(u)^N &= \Delta t \left( \frac{1}{2} u^N + \lambda^N \right)\end{aligned}$$

Lets try to understand what happens for  $n = 0$  and  $n = N$ . For  $n = 0$  we see that there is no  $\lambda$  term. This is because  $y$  does not depend on  $u(0)$ . The reason that this matters in the discrete case and not in the continuous case, is that the point  $t = 0$  has measure zero, and the continuous gradient is an integral. We also notice the  $\frac{1}{2}$  term in front off  $\Delta t u^0$ . This comes from our numerical integration using the trapezoidal rule. To make this clear lets state the trapezoidal rule:

$$\int_0^1 f(t)dt \approx \Delta t \left[ \frac{f^0 + f^N}{2} + \sum_{n=1}^{N-1} f^n \right]$$

Looking at this expression we also understand the  $n = N$  case. Also note that integrating over  $(\lambda + \frac{1}{2}u)e^N$  using the trapezoidal rule would give us an extra factor of  $\frac{1}{2}$  that is not there when we use finite difference for  $\hat{J}'(u)$ . This Will all be demonstrated below. One could perhaps derive the discrete results by translating the functional and the ODE to discrete setting , where you exchange  $L^2(\Omega)$  with  $\mathbb{R}^{N+1}$ , but I will not do this now.

### Testing numerics with simple example

Want to test the numerical adjoint to the exact adjoint for the simple example I did above, i.e.  $T = y_T = y_0 = \alpha = 1$  and  $u = 0$ . This gave us the the following solution to our adjoint equation:  $\lambda(t) = (e - 1)e^{1-t}$ . Using the finite difference schemes I derived above, I calculated the maximum difference between the exact and the numerical adjoint for  $N = \{50, 100, 500, 1000\}$  points. The results of the experiment is added in the table below:

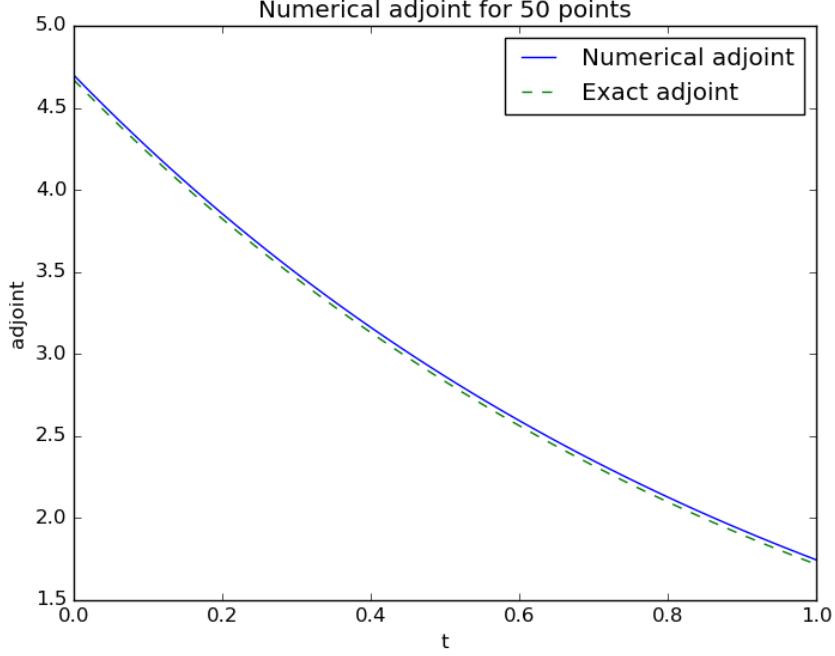


Figure 1: Adjoint for  $u = 0$  and  $T = y_T = y_0 = \alpha = 1$

N	50	100	500	1000
$\max( \lambda^n - \lambda(t^n) )$	0.0317	0.0156	0.0031	0.0015

Using least squares we can find the convergence rate of  $|\lambda^n - \lambda(t^n)|$  in  $\Delta t$ , and as expected using simple backward Euler, we get linear convergence:

$$|\lambda^n - \lambda(t^n)|_\infty \leq \Delta t C$$

In this case  $C \approx 1.7$ . I have also added a plot of the exact and numerical adjoints for  $N = 50$ .

### Testing gradient using finite difference

Now lets try to test the claims I made earlier about the discrete gradient. I will approximate the gradient using finite difference in the following way:

$$\hat{J}'(u)^n \approx \frac{\hat{J}(u + \epsilon^n) - \hat{J}(u)}{\epsilon}$$

$\epsilon^n = \epsilon e^n \in \mathbb{R}^{N+1}$  with  $\epsilon > 0$  small, and  $e^n$  the unit vector

As always I let  $T = y_T = y_0 = \alpha = 1$ , however this time I choose  $u(t) = e^t + t$ . I then define the relative error E between the discrete adjoint gradient  $\hat{J}'_{\Delta t}(u)$

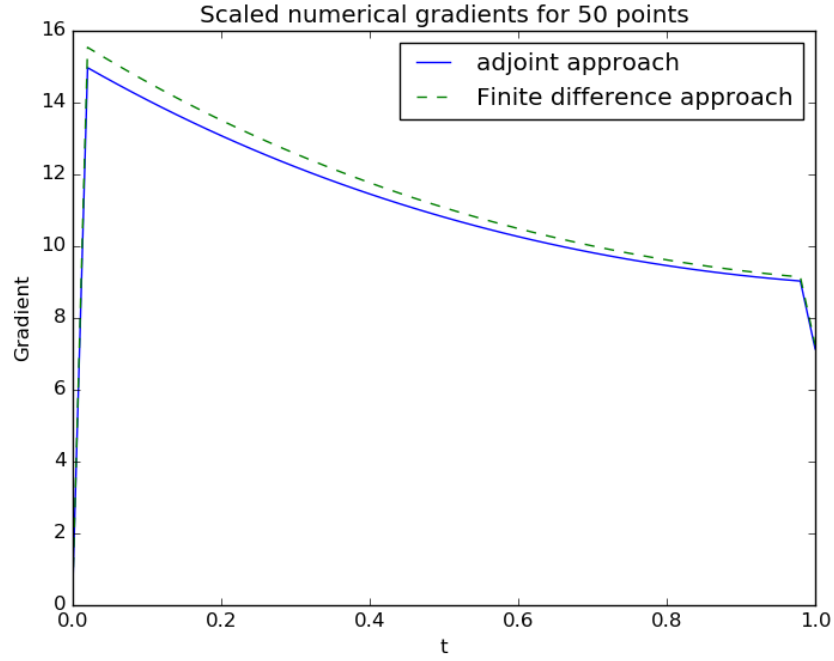


Figure 2: "Relative" gradients for  $u = 0$  and  $T = y_T = y_0 = \alpha = 1$

and the finite difference gradient  $\hat{J}'_\epsilon(u)$  defined as:

$$E = \left| \frac{\hat{J}'_{\Delta t}(u) - \hat{J}'_\epsilon(u)}{\Delta t} \right|_\infty$$

I use this error to test the gradients for different  $N$ . The result is given in a table below, and I have also added a plot. Note that I as last time calculated convergence rate using least squares, and the result was:  $E \leq \Delta t C$ , with  $C \approx 27$ .

N	50	100	500	1000
E	0.5658	0.2816	0.0561	0.0281