Individual Sections of the Book

Inverse Problems: Exercices

With mathematica, matlab, and scilab solutions

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### 8.3 Second Derivative Operators and their Transposes

The finite-difference approximation to the second derivative can be obtained by applying twice the first derivative (equation 8.2). This gives

\[
\ddot{p}(t) = \frac{p(t + 2\Delta t) - 2p(t) + p(t - 2\Delta t)}{(2\Delta t)^2},
\]

(8.36)

or, for discretized functions,

\[
\ddot{p}_i = \frac{p_{i+2} - 2p_i + p_{i-2}}{(2\Delta t)^2}.
\]

(8.37)

If the application one has in mind involves both, first and second derivatives, these are the right starting equations. But if, as in the application below (wave equation), one has to deal only with second derivatives, one can as well redefine the \(\Delta t\), and write equation 8.36 as

\[
\ddot{p}(t) = \frac{p(t + \Delta t) - 2p(t) + p(t - \Delta t)}{\Delta t^2},
\]

(8.38)

i.e., for discretized functions,

\[
\ddot{p}_i = \frac{p_{i+1} - 2p_i + p_{i-1}}{\Delta t^2}.
\]

(8.39)

Solving equation 8.38 for \(p(t + \Delta t)\) first, then for \(p(t - \Delta t)\), and redefining \(t\), gives the two relations

\[
p(t) = 2p(t - \Delta t) - p(t - 2\Delta t) + \Delta t^2 \ddot{p}(t - \Delta t)
\]

\[
p(t) = 2p(t + \Delta t) - p(t + 2\Delta t) + \Delta t^2 \ddot{p}(t + \Delta t)
\]

(8.40)

i.e., for discretized functions,

\[
p_i = 2p_{i-1} - p_{i-2} + \Delta t^2 \ddot{p}_{i-1}
\]

\[
p_i = 2p_{i+1} - p_{i+2} + \Delta t^2 \ddot{p}_{i+1}
\]

(8.41)

While equation 8.39 is to be used for computing second derivatives, the two equations 8.41 are to be used for computing second primitives, respectively when initial or final conditions are given.

There are different second-derivative operators to be considered, depending on the type of boundary conditions used. Typically, when the derivatives are with respect to time, one considers two initial conditions or two final conditions, while when the derivatives are with respect to a space variable one considers one condition at each side (that may be a free boundary condition or a rigid boundary condition).

#### 8.3.1 Time Derivatives

One may start by considering a \(k\)-dimensional space \(\mathbb{P}\), and by considering that the second derivative operator maps the \(k\) quantities \(\{p_0, p_1, p_2, \ldots, p_{k-1}\}\) into the \(k\) quantities
\{\dot{p}_1, \dot{p}_2, \ldots, \dot{p}_{k-2}\}, but seen in that way, the second derivative has not an inverse, so let us instead consider the \(k - 2\)-dimensional subspace of \(\mathbf{P}\) corresponding to the initial conditions of rest

\[
p_0 = 0 \quad ; \quad p_1 = 0 .
\]

We shall denote this space \(\overrightarrow{\mathbf{P}}\). Its elements are of the form \(\mathbf{p} = \{p_2, p_3, \ldots, p_{k-2}, p_{k-1}\}\). We introduce the second derivative operator \(\overrightarrow{\mathbf{D}}^2\) through its matrix representation:

\[
\begin{pmatrix}
\dot{p}_1 \\
\dot{p}_2 \\
\dot{p}_3 \\
\dot{p}_4 \\
\vdots \\
\dot{p}_{k-4} \\
\dot{p}_{k-3} \\
\dot{p}_{k-2}
\end{pmatrix} = \frac{1}{\Delta t^2}
\begin{pmatrix}
+1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
-2 & +1 & 0 & 0 & \cdots & 0 & 0 & 0 \\
+1 & -2 & +1 & 0 & \cdots & 0 & 0 & 0 \\
0 & +1 & -2 & +1 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
p_2 \\
p_3 \\
p_4 \\
p_5 \\
\vdots \\
p_{k-3} \\
p_{k-2} \\
p_{k-1}
\end{pmatrix}
\]

\(8.43\)

For short, we write

\[
\mathbf{\ddot{p}} = \overrightarrow{\mathbf{D}}^2 \mathbf{p} .
\]

\(8.44\)

The operator \(\overrightarrow{\mathbf{D}}^2\) maps the \((k - 2)\)-dimensional space \(\overrightarrow{\mathbf{P}}\) into a \((k - 2)\)-dimensional space \(\overrightarrow{\mathbf{P}}\) made of strings having the form \(\{\ddot{p}_1, \ddot{p}_2, \ldots, \ddot{p}_{k-2}\}\) (see figures 8.4 and 8.5).

Figure 8.4: Note: explain that these are the different operators implemented in this section.

The action of \(\overrightarrow{\mathbf{D}}^2\) on a vector \(\mathbf{p} \in \overrightarrow{\mathbf{P}}\) is not computed using matrix multiplication, but,
Figure 8.5: The two derivative operators $\overrightarrow{D}^2$ and $\overleftarrow{D}^2$ introduced in the text, as well as their inverses, the integral operators $\overrightarrow{D}^{-2}$ and $\overleftarrow{D}^{-2}$. The space $\overrightarrow{Q}$ can be identified with the dual of $\overrightarrow{P}$ while $\overleftarrow{Q}$ can be identified with the dual of $\overleftarrow{P}$. The covariance operator $C_{\overrightarrow{Q}}$ maps $\overrightarrow{P}$ into its dual $\overrightarrow{Q}$ (see below), while the covariance operator $C_{\overleftarrow{Q}}$ maps $\overleftarrow{Q}$ into its dual $\overleftarrow{P}$. Note: explain that all spaces have dimension $k - 2$. 

\begin{align*}
(p_0 = 0, p_1 = 0) & \quad \overrightarrow{D}^2 \quad (\text{2nd. derivative}) \\
q_{k+1} = 0, q_k = 0 & \quad \overleftarrow{D}^{-2} \quad (\text{2nd. integral})
\end{align*}
rather, via the algorithm

\[
\begin{align*}
\dot{p}_i &= (p_{i+1} - 2p_i + p_{i-1})/\Delta t^2 & I \in \{3, 5, \ldots, 2k-1\} \\
\ddot{p}_2 &= (p_3 - 2p_2 + 0)/\Delta t^2 & (p_1 \text{ undefined, value assumed to be zero}) \\
\ddot{p}_1 &= (p_2 - 20 + 0)/\Delta t^2 & (p_0 \text{ undefined, value assumed to be zero})
\end{align*}
\]

the operations being performed in any order.

Note: explain here that the inverse of relation 8.43 is easy to obtain:

\[
\begin{align*}
(p_0 = 0) \\
(p_1 = 0) \\
\begin{pmatrix}
p_2 \\
p_3 \\
p_4 \\
p_5 \\
\vdots \\
p_{k-3} \\
p_{k-2} \\
p_{k-1}
\end{pmatrix} = \Delta t^2
\begin{pmatrix}
1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
2 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\
3 & 2 & 1 & 0 & \cdots & 0 & 0 & 0 \\
4 & 3 & 2 & 1 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
k-2 & \cdots & \cdots & \cdots & \cdots & 1 & 0 & 0 \\
k-1 & k-2 & \cdots & \cdots & \cdots & 2 & 1 & 0 \\
k & k-1 & k-2 & \cdots & \cdots & 3 & 2 & 1
\end{pmatrix}
\begin{pmatrix}
\dddot{p}_1 \\
\dddot{p}_2 \\
\dddot{p}_3 \\
\dddot{p}_4 \\
\vdots \\
\dddot{p}_{k-4} \\
\dddot{p}_{k-3} \\
\dddot{p}_{k-2}
\end{pmatrix} \quad (p_0 = 0) \quad (p_1 = 0)
\end{align*}
\]

(8.46)

Note: refer here to figure 8.6

\[p = \mathbf{D}^{-2} \dddot{p}\]

\[q = \mathbf{D}^{-2} \dddot{q}\]

Figure 8.6: Note: explain that these are the different operators implemented in this section.

As above, the algorithmic implementation of the second integral operator \(\mathbf{D}^{-2}\) is not
done via matrix multiplication: when the input is the \(k\)-dimensional string \(\{\dddot{p}_1, \dddot{p}_2, \ldots, \dddot{p}_{k-2}\}\),
the output is the \(k\)-dimensional string \(\{p_2, p_3, \ldots, p_{k-1}\}\), computed, in fact, via the recursive
algorithm

\[
\begin{align*}
    p_2 &= \Delta t^2 \ddot{p}_1 \quad (p_0 \text{ and } p_1 \text{ undefined, values assumed to be zero}) \\
    p_3 &= 2p_2 + \Delta t^2 \ddot{p}_2 \quad (p_1 \text{ undefined, value assumed to be zero}) \\
    p_4 &= 2p_3 - p_2 + \Delta t^2 \ddot{p}_3 \\
    \vdots &= \vdots \\
    p_{k-2} &= 2p_{k-3} - p_{k-4} + \Delta t^2 \ddot{p}_{k-3} \\
    p_{k-1} &= 2p_{k-2} - p_{k-3} + \Delta t^2 \ddot{p}_{k-2} 
\end{align*}
\]  

(8.47)

each term of it being obviously consistent with the first of equations 8.41.

Note: introduce here the second matrix representation of the finite-difference approximation to the second derivative is (for functions satisfying final conditions of rest)

\[
\begin{pmatrix}
    \ddot{q}_2 \\
    \ddot{q}_3 \\
    \ddot{q}_4 \\
    \ddot{q}_5 \\
    \vdots \\
    \ddot{q}_{k-1} \\
    \ddot{q}_k \\
    \ddot{q}_{k+1}
\end{pmatrix} = \frac{1}{\Delta t^2} \begin{pmatrix}
    1 & -2 & 1 & 0 & \cdots & 0 & 0 & 0 \\
    0 & 1 & -2 & 1 & \cdots & 0 & 0 & 0 \\
    0 & 0 & 1 & -2 & \cdots & 0 & 0 & 0 \\
    \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
    0 & 0 & 0 & 0 & \cdots & 1 & -2 & 1 \\
    0 & 0 & 0 & 0 & \cdots & 0 & 1 & -2 \\
    0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 
\end{pmatrix} \begin{pmatrix}
    q_1 \\
    q_2 \\
    q_3 \\
    q_4 \\
    \vdots \\
    q_{k-2} \\
    q_{k-1} \\
    q_k 
\end{pmatrix} \\
\begin{pmatrix}
    (q_{k+1} = 0) \\
    (q_{k+2} = 0)
\end{pmatrix} 
\]  

(8.48)

For short,

\[
\ddot{q} = \overrightarrow{D}^2 \dot{q} 
\]  

(8.49)

Note: write here the algorithm.

Note: give here the inverse operator.

Note: explain here that, as the matrix representing \( \overrightarrow{D}^2 \) is the transpose of that representing \( \overleftarrow{D}^2 \), the matrix representing \( \overrightarrow{D}^{-2} \) is, of course, the transpose of the matrix in equation 8.46.

Note: this is old text: Consider a second \( k - 2 \)-dimensional space \( \mathcal{Q} \) made of functions \( \ddot{q} = \{\ddot{q}_2, \ddot{q}_3, \ldots, \ddot{q}_{k-1}\} \). This space can be considered the dual of \( \mathcal{P} \)

\[
\mathcal{Q} = ^*\mathcal{P} 
\]  

(8.50)

in the sense that if one element \( \dot{p} \in \mathcal{P} \) and one element \( \ddot{q} \in \mathcal{Q} = ^*\mathcal{P} \) are given, we associate to them their duality product, defined as the scalar quantity

\[
\langle \ddot{q}, \dot{p} \rangle = \sum_{i=\{2,3,\ldots,k-1\}} \ddot{q}_i \dot{p}_i 
\]  

(8.51)
We need two more spaces. The space \( \mathbf{\dot{P}} \) has also \( k-2 \) dimensions, and is made of functions \( \dot{p} = \{ \dot{p}_1, \dot{p}_2, \ldots, \dot{p}_{k-2} \} \). Finally, assuming that \( q_{k-1} \) and \( q_k \) are two fixed quantities, the \( k-2 \)-dimensional space \( \mathbf{Q} \) is made of functions \( q = \{ q_1, q_2, \ldots, q_{k-2}, [q_{k-1}], [q_k] \} \), where the other \( k-2 \) quantities are variable. This space \( \mathbf{Q} \) can be considered to be the dual of \( \mathbf{\dot{P}} \)

\[
\mathbf{Q} = \ast \mathbf{\dot{P}},
\]

because if one element \( \dot{p} \in \mathbf{A} \) and one element \( q \in \mathbf{A}^* \) are given, we associate to them their duality product

\[
\langle q, \dot{p} \rangle = \sum_{I=\{k-2,k-3,\ldots,1\}} q_I a_I.
\]

The first of the second-derivative operators, that we shall denote \( \mathbf{\ddot{D}}^2 \), goes from \( \mathbf{\dot{P}} \) into \( \mathbf{\ddot{P}} \), and is defined via (this is equation 8.39, with the indices explicited)

\[
\dot{p}_I = \frac{p_{I+1} - 2 p_I + p_{I-1}}{\Delta t^2}; \quad I = \{k-2,k-3,\ldots,1\},
\]

an expression that we symbolically write

\[
\dot{p} = \mathbf{\ddot{D}}^2 p.
\]

The order chosen here for the variation of the index (from the largest to the smallest) is not important: it is just for consistency with the integral operator (so the index \( I \) always runs in the same sense). We can now introduce another second-derivative operator, that we shall denote \( \mathbf{\dddot{D}}^2 \), that goes from \( \mathbf{Q} \) into \( \mathbf{\ddot{P}} \), and that is defined via (again, this is equation 8.39, with the indices explicited)

\[
\ddot{q}_i = \frac{q_{i+1} - 2 q_i + q_{i-1}}{\Delta t^2}; \quad i = \{2,3,\ldots,k-1\},
\]

an expression that we symbolically write

\[
\ddot{q} = \mathbf{\dddot{D}}^2 q.
\]

Let us now demonstrate that if the initial and final values of the considered functions are related via a constraint (to be found during the demonstration), the operator \( \mathbf{\ddot{D}}^2 \) is the transpose of \( \mathbf{\dddot{D}}^2 \) (i.e., loosely speaking, that the second-derivative operator is symmetric). Using the abstract definition of transpose (already mentioned in the previous section), what we have to demonstrate is that for any \( p \in \mathbf{P} \) and for any \( q \in \mathbf{Q} \), one has

\[
\langle q, \mathbf{\ddot{D}}^2 p \rangle = \langle \mathbf{\dddot{D}}^2 q, p \rangle.
\]

Using the two definitions 8.51 and 8.53 for the duality product, and the two definitions 8.54 and 8.56 for the second derivatives, we obtain a sum of terms, that all cancel each other, excepted six of them, so the condition 8.58 becomes

\[
p_0 q_1 + p_1 (q_2 - 2 q_1) = q_k p_{k-1} + q_{k-1} (p_{k-2} - 2 p_{k-1})
\]

Again, we find a relation between the initial and the final values of the functions. As mentioned above, these kind of conditions are called dual boundary conditions.

We have thus arrived at the following...
Property 8.1 When the functions \( p \) on which the second-derivative operator \( \overrightarrow{D}^2 \) (introduced in equation 8.59) is applied, and the functions \( q \) on which the second-derivative operator \( \overleftarrow{D}^2 \) (introduced in equation 8.59) is applied, satisfy the general dual boundary condition in equation 8.59 (a fortiori, if they satisfy the special dual boundary condition in equation 8.61), then \( \overrightarrow{D}^2 \) is the transpose of \( \overleftarrow{D}^2 \):

\[
(\overrightarrow{D}^2)^t = \overleftarrow{D}^2 .
\]

The obvious example where the dual boundary conditions 8.59 are satisfied is

\[
p_0 = p_1 = 0 ; \quad q_k = q_{k-1} = 0 .
\]

Note that these equations can also be read as saying that both, the functions and their (first) derivatives are zero (at the beginning for \( p \), and at the end for \( q \)). If \( p_0 \) and/or \( p_1 \) are not zero, then, one needs to create a suitable \( q \). This can be done as follows. Note: I have to simplify a lot the text in the footnote.

The two operators \( \overrightarrow{D}^2 \) and \( \overleftarrow{D}^2 \) have inverses, that are second integrals. The can easily be obtained from equations 8.41, but let us write them explicitly, caring to use the right indices. Given the two fixed values \( p_0 \) and \( p_1 \), and the \( k \) variable quantities \( \{a_1, a_2, \ldots, a_{k-2}\} \) the operator \( \overrightarrow{D}^{-2} \) produces the \( k \) quantities

\[
p_i = 2p_{i-1} - p_{i-2} + \Delta t^2 a_{i-1} ; \quad i = \{2,3,\ldots,k-1\} .
\]

Of course, the \( p \) so obtained is the second primitive of \( a \) that satisfies the given double initial condition. Clearly, this operator \( \overrightarrow{D}^{-2} \) defines a mapping from \( \mathbb{P} \) into \( \mathbb{P} \). Similarly, given the two fixed values \( q_k \) and \( q_{k-1} \), and the \( k \) variable quantities \( \{\bar{q}_2, \bar{q}_3, \ldots, \bar{q}_{k-1}\} \) the operator \( \overleftarrow{D}^{-2} \) produces the \( k \) quantities

\[
q_l = 2q_{l+1} - q_{l+2} + \Delta t^2 \bar{q}_{l+1} ; \quad l = \{k-2, \ldots, 2, 1\} .
\]

Of course, the \( p \) so obtained is the second primitive of \( a \) that satisfies the given double final condition. This operator \( \overleftarrow{D}^{-2} \) defines a mapping from \( \mathbb{Q} = \mathbb{P} \) into \( \mathbb{Q} = \mathbb{P} \).

8.3.2 Computer Implementation of the Second Derivative Operators

Executable notebook at

http://www.ipgp.jussieu.fr/~tarantola/exercices/chapter_08/DualitySecondDerivative.nb

Let us now implement the operators we have just defined. As in the previous section, we will do this while checking that we do have transpose operators (note: explain this).

We start by defining a time interval and a time step,

\[\text{Given an (arbitrary) function } a = \{a_1, a_2, \ldots, a_{k-1}\}, \text{ and the two (arbitrary) initial values } p_0 \text{ and } p_1, \text{ we can evaluate, by double forward integration, the function } \mathbf{p} = \{p_2, p_3, \ldots, p_{k-1}\}. \text{ This, is particular, produces the two values } p_{k-2} \text{ and } p_{k-1} \text{ that appear in the duality condition 8.59. Then, given an (arbitrary) function } \mathbf{q} = \{q_2, q_3, \ldots, q_{k-1}\}, \text{ and given the two final conditions } q_k = 0 \text{ and } q_{k-1} = 0, \text{ we evaluate, by double backwards integration, the function } \{\bar{q}_{k-2}, \bar{q}_{k-3}, \ldots, \bar{q}_1\}. \text{ Of course, the function } \mathbf{q'} \text{ so obtained will generally not satisfy the duality condition. But, if } q' = \{q'_2, q'_3, \ldots, q'_{k-2}, [q'_{k-1} = 0], [q'_k = 0]\} \text{ is a double primitive of } \mathbf{q}, \text{ so it will be the function } \mathbf{q} \text{ obtained by adding a constant value } p \text{ to all the components of } \mathbf{q'}, \text{ and we only need to use the value of } p \text{ such that the function } \mathbf{q} \text{ satisfies the duality condition. A simple computation gives } p = (p_0 q'_1 + p_1 (q'_2 - 2q'_1))/((p_1 - p_0) - (p_{k-1} - p_{k-2})).\]
8.3 Second Derivative Operators and their Transposes

(* Definition of the grid *)
tmin = 0.; tmax = 12.; k = 241;
dt = (tmax-tmin)/(k-1);

we chose an arbitrary function \( f(t) \), and discretize it, this defining the function \( p \)

(* Choice of an arbitrary function, and its discretization *)
f[t_] := (1-Cos[t]) - ((dt/2)^2/2)
Do[ p[i] = f[(i-1/2) dt] , {i,0,k-1} ]

(the function \( f(t) \) is such that \( p_0 = p_1 = 0 \)). We implement the second derivative operator \( \dddot{p} = \overrightarrow{D^2} p \):

(* Second derivative operator (I) *)
Do[ pdd[i] = (p[i+1] - 2 p[i] + p[i-1]) / dt^2 , {i,1,k-2} ]

This gives the discretized version of the second derivative of \( f(t) \). We chose a second arbitrary function \( g(t) \), and discretize it, this defining the function \( q \),

(* Choice of an arbitrary function, and its discretization *)
g[t_] := (t-12.)^2 - (dt/2)^2
Do[ q[i] = g[(i-1/2) dt] , {i,k,1,-1} ]

(the function \( q(t) \) is such that \( q_k = q_{k-1} = 0 \)). We implement the second derivative operator \( \dddot{q} = \overleftarrow{D^2} q \):

(* Second derivative operator (II) *)
Do[ qdd[i] = (q[i+1] - 2 q[i] + q[i-1]) / dt^2 , {i,k-1,2,-1} ]

We compute the first duality product

(* Duality product (I) *)
duality2 = Sum[ qdd[i] p[i] , {i,2,k-1} ]

and the second duality product

(* Duality product (II) *)
duality1 = Sum[ q[i] pdd[i] , {i,1,k-2} ]

Within machine accuracy, these two numbers are identical (501.315), as they should.

8.3.3 Computer Implementation of the Second Integral Operators

Executable notebook at
http://www.ipgp.jussieu.fr/~tarantola/exercices/chapter_08/DualitySecondDerivative.nb

Bla, bla, bla...

Bla, bla, bla...

Computing the second forward primitive of \( \dddot{p} \),
we obtain a function that, within machine accuracy, is identical to \( p \). Computing the second backward primitive of \( \ddot{q} \),

\[
(* \text{ Backward integral operator } *)
\]

\[
\text{Do[ } qq[I] = 2 \cdot qq[I+1] - qq[I+2] + dt^2 \cdot qdd[I+1] , \{I, k-2, 1, -1\} \text{ ]}
\]

we obtain a function that, within machine accuracy, is identical to \( q \).

Note: I need to implement \( \Delta \).

### 8.3.4 Space Derivatives (1D Laplacian)

Our example (one free boundary, one rigid boundary):

\[
\begin{pmatrix}
    p''_1 \\
    p''_2 \\
    p''_3 \\
    p''_4 \\
    \vdots \\
    p''_{\ell-2} \\
    p''_{\ell-1} \\
    p''_{\ell}
\end{pmatrix}
= \frac{1}{\Delta t^2}
\begin{pmatrix}
    -2 & +1 & 0 & 0 & \cdots & 0 & 0 & 0 \\
    +1 & -2 & +1 & 0 & \cdots & 0 & 0 & 0 \\
    0 & +1 & -2 & +1 & \cdots & 0 & 0 & 0 \\
    0 & 0 & +1 & -2 & \cdots & 0 & 0 & 0 \\
    \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
    0 & 0 & 0 & 0 & \cdots & -2 & +1 & 0 \\
    0 & 0 & 0 & 0 & \cdots & +1 & -2 & +1 \\
    0 & 0 & 0 & 0 & \cdots & 0 & +1 & -1
\end{pmatrix}
\begin{pmatrix}
    p_0 \\
    p_1 \\
    p_2 \\
    p_3 \\
    p_4 \\
    \vdots \\
    p_{\ell-2} \\
    p_{\ell-1} \\
    p_{\ell}
\end{pmatrix}
\]

\[
(p_0 = 0)
\]

(8.64)

For short,

\[
p'' = \Delta p
\]

(8.65)

When the second derivative under examination is with respect to the time variable, one typically faces the two cases already examined, when one has two initial conditions or two final conditions. But when the derivatives are with respect to a space variable, one typically faces a third situation where one has two boundary conditions, one “at the left” and the other “at the right”. We still have to analyze this situation in detail. In order to distinguish this spatial second-derivative operator from the temporal second-derivative operators introduced above, let us denote it with the symbol \( \Delta \). Also, let us replace the symbol \( k \), that was above related with the dimension of the spaces by the symbol \( \ell \) (space strings and time string have typically different lengths).
Figure 8.7: Note: explain that these are the different operators implemented in this section.

Figure 8.8: The two derivative operators $\Delta$ and ...
Instead of introducing new notations for the new spaces, let us use the same notations used above, slightly altering the definitions. All the spaces have here dimension $\ell - 1$. The first space, now, is the $\mathbf{P}$ is made of functions $p = \{[p_0], p_1, p_2, \ldots, p_{\ell-1}, [p_{\ell}]\}$, where the two quantities $p_0$ and $p_{\ell}$ are fixed, and the other $\ell - 1$ quantities are variable (see figure 8.7). We introduce another $\ell - 1$-dimensional space $\mathbf{Q}''$ is made of functions $q'' = \{q''_1, q''_2, \ldots, q''_{\ell-1}\}$. This space can be considered to be the dual of $\mathbf{P}$,

$$Q'' = P$$

(8.66)
as if one element $p \in \mathbf{P}$ and one element $q'' \in \mathbf{Q}$ are given, we can associate to them their duality product, defined as the scalar quantity

$$\langle q'', p \rangle = \sum_{i \in \{1, 2, \ldots, \ell - 1\}} q''_i p_i$$

(8.67)

Another space, $\mathbf{P}''$, is made of functions $p'' = \{p''_1, p''_2, \ldots, p''_{\ell-1}\}$, and the final space, $\mathbf{Q}'$, is now made of functions $q = \{[q_0], q_1, q_2, \ldots, q_{\ell-1}, [q_{\ell}]\}$, where the two quantities $q_0$ and $q_{\ell}$ are fixed, and the other $\ell - 1$ quantities are variable. The space $\mathbf{Q}$ is the dual of $\mathbf{P}''$, $\mathbf{Q} = P''$,

(8.68)

with the duality product

$$\langle q, p'' \rangle = \sum_{i \in \{1, 2, \ldots, \ell - 1\}} q_i p''_i$$

(8.69)

The second-derivative operator $\Delta$ goes from $\mathbf{P}$ into $\mathbf{P}''$, and is defined via

$$p''_I = \frac{p_{I+1} - 2p_I + p_{I-1}}{\Delta t^2} ; \quad I = \{1, 2, \ldots, \ell - 1\}$$

(8.70)
an expression that we symbolically write

$$p'' = \Delta p .$$

(8.71)

We introduce another second-derivative operator, that we provisionally denote $\Delta'$, that goes from $\mathbf{Q} = P''$ into $\mathbf{Q}'' = *P$, and that is defined via

$$q''_i = \frac{q_{i+1} - 2q_i + q_{i-1}}{\Delta t^2} ; \quad i = \{1, 2, \ldots, \ell - 1\}$$

(8.72)
an expression that we symbolically write

$$q'' = \Delta' q .$$

(8.73)

Let us now demonstrate that the operator $\Delta'$ just introduced is the transpose of $\Delta$ (from where the notation). Similarly to what we did above, we need to demonstrate that for any $p \in \mathbf{P}$ and for any $q \in \mathbf{Q}$, one has

$$\langle q, \Delta' p \rangle = \langle \Delta' q, p \rangle$$

(8.74)

This requirement leads now to the condition

$$p_0 q_1 - p_1 q_0 = q_{\ell} p_{\ell-1} - q_{\ell-1} p_{\ell} .$$

(8.75)

Therefore, we have the following
8.3 Second Derivative Operators and their Transposes

**Property 8.2** When the vectors \( p \) on which the second-derivative operator \( \Delta \) is applied, and the vectors \( q \) on which the second-derivative operator \( \Delta^t \) is applied, satisfy the general dual boundary condition in equation 8.75 (a fortiori, the special dual condition in equation 8.76), then \( \Delta^t \) is the transpose of \( \Delta \) (from where the notation).

The first example where the dual boundary condition 8.75 is satisfied is

\[
p_0 = 0 \quad , \quad q_0 = 0 \quad ; \quad p_\ell = 0 \quad , \quad q_\ell = 0 \quad . \tag{8.76}
\]

Here, the functions \( p \) and \( q \) satisfy both a “free condition” at the right and at the end. The second example where the dual boundary condition 8.75 is satisfied is

\[
p_0 = p_1 \quad ; \quad p_\ell = p_\ell-1 \quad ; \quad q_0 = q_1 \quad ; \quad q_\ell = q_\ell-1 \quad . \tag{8.77}
\]

Here, the functions \( p \) and \( q \) satisfy both a “rigid condition” at the right and at the end. We see that the difference between the second-derivative operator \( \Delta \) and the second-derivative operator \( \Delta^t \) is so subtle, that we can just use same notation \( \Delta \) for both.