Analytic Regularization

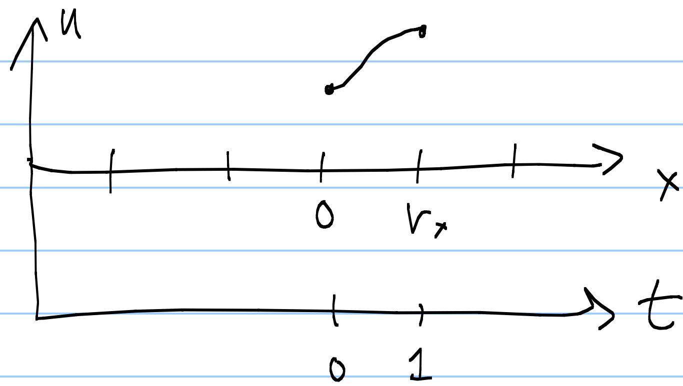
Note Title 5/22/2010

Consider the second derivative regularization score:

$$S = \int \left(\frac{\partial u_x}{\partial x^2}\right)^2 + \left(\frac{\partial u_x}{\partial y^2}\right)^2 + \left(\frac{\partial u_x}{\partial z^2}\right)^2$$
$$+ \left(\frac{\partial u_x}{\partial x \partial y}\right)^2 + \left(\frac{\partial u_x}{\partial x \partial z}\right)^2 + \left(\frac{\partial u_x}{\partial y \partial z}\right)^2$$
$$+ \left(\frac{\partial u_y}{\partial x^2}\right)^2 + \cdots$$

Our goal is to find an expression for S that we can compute.

Let's look at it in 1-D $\int_0^1 \left(\frac{\partial^2 u}{\partial x^2}\right)^2$



We solve for $\partial u / \partial x$, $\partial^2 u / \partial x^2$

$$u(x) = p^T B t$$

where
$$p = \begin{bmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \end{bmatrix} \quad B = \frac{1}{6}\begin{bmatrix} 1 & 4 & 3 & -1 \\ -3 & 0 & -6 & 3 \\ 1 & 3 & 3 & -3 \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad t = \begin{bmatrix} 1 \\ t \\ t^2 \\ t^3 \end{bmatrix}$$

Or, in terms of x,
$$t = \begin{bmatrix} 1 \\ x/r_x \\ x^2/r_x^2 \\ x^3/r_x^3 \end{bmatrix}$$

where r_x is the grid spacing.

If we let
$$R \triangleq \begin{bmatrix} 1 & & & \\ & 1/r_x & & \\ & & 1/r_x^2 & \\ & & & 1/r_x^3 \end{bmatrix},$$

we have
$$u(x) = p^T B R \begin{bmatrix} 1 \\ x \\ x^2 \\ x^3 \end{bmatrix}$$

Let $q^T \triangleq p^T B R$. Then

$$\frac{\partial u}{\partial x} = q^T \begin{bmatrix} 0 \\ 1 \\ 2x \\ 3x^2 \end{bmatrix} \qquad \frac{\partial^2 u}{\partial x^2} = q^T \begin{bmatrix} 0 \\ 0 \\ 2 \\ 6x \end{bmatrix}.$$

$$\left(\frac{\partial^2 u}{\partial x^2}\right)^2 = q^T \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 12x \\ 0 & 0 & 12x & 36x^2 \end{bmatrix} q$$

$$\int_0^1 \left(\frac{\partial^2 u}{\partial x}\right)^2 = q^T \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 4x & 6x^2 \\ 0 & 0 & 6x^2 & 12x^3 \end{bmatrix} q \Bigg|_0^1$$

$$= q^T \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 6 \\ 0 & 0 & 6 & 12 \end{bmatrix} q.$$

Next, consider the 3-D case.

$$u_x(x,y,z) = \sum_i \sum_j \sum_k p_{ijk} \, B_i(x) B_j(y) B_k(z)$$

We will take as example:

$$\int_0^1\int_0^1\int_0^1 \left(\frac{\partial^2 u_x}{\partial x \partial y}\right)^2 dx\,dy\,dz$$

Let $\quad x = \begin{bmatrix} 1 \\ x \\ x^2 \\ x^3 \end{bmatrix}$

$$u_x(x,y,z) = \sum_{ijk} p_{ijk} \left(\sum_a B(i,a) R_x(a) \, x(a) \right)$$

$$\cdot \left(\sum_b B(j,b) R_y(b) \, y(b) \right) \cdot \left(\sum_c B(k,c) R_z(c) \, z(c) \right)$$

Let $\Delta^{(1)} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 3 & 0 \end{bmatrix}$

$\Delta^{(2)} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 \end{bmatrix}$

Let $Q_x^{(\delta)} \triangleq B R_x \Delta^{(\delta)}$

$$u_x(x,y,z) = \sum_{ijk} P_{ijk} \left(\sum_a Q_x^{(0)}(i,a)\, x(a) \right) \cdot \left(\sum_b Q_y^{(0)}(j,b)\, y(b) \right) \cdot \left(\sum_c Q_z^{(0)}(k,c)\, z(c) \right)$$

$$\frac{\partial u}{\partial x} = \sum_{ijk} P_{ijk} \left(\sum_a Q_x^{(1)}(i,a)\, x(a) \right) \cdot \left(\sum_b Q_y^{(0)}(j,b)\, y(b) \right) \cdot \left(\sum_c Q_z^{(0)}(k,c)\, z(c) \right)$$

$$\frac{\partial^2 u}{\partial x \partial y} = \sum_{ijk} P_{ijk} \left(\sum_a Q_x^{(1)}(i,a)\, x(a) \right)$$

$$\cdot \left(\sum_b Q_y^{(1)}(j,b)\, y(b) \right) \cdot \left(\sum_c Q_z^{(0)}(k,c)\, z(c) \right)$$

$$\left(\frac{\partial^2 u}{\partial x \partial y} \right)^2 = P^T \left(v\, v^T \right) P = p^T V p$$

where

$$p = \begin{bmatrix} p_{111} \\ p_{112} \\ \vdots \\ \\ p_{444} \end{bmatrix}, \quad v = \begin{bmatrix} v_{111} \\ v_{112} \\ \vdots \\ \\ v_{444} \end{bmatrix}, \text{ and}$$

where $v_{ijk} = \left(\sum_a Q_x^{(1)}(i,a)\, x(a) \right)$

$$\cdot \left(\sum_b Q_y^{(1)}(j,b)\, y(b) \right) \cdot \left(\sum_c Q_z^{(0)}(k,c)\, z(c) \right)$$

$$\int_0^1\int_0^1\int_0^1 \left(\frac{\partial^2 u}{\partial x \partial y}\right)^2 = \iiint p^T V p = p^T \left(\iiint V\right) p$$

$$V(d,e) = v_{ijk} \cdot v_{lmn}$$

$$= \left(\sum_a Q_x^{(1)}(i,a)\, x(a)\right)$$

$$\cdot \left(\sum_b Q_y^{(1)}(j,b)\, y(b)\right)$$

$$\cdot \left(\sum_c Q_z^{(0)}(k,c)\, z(c)\right)$$

$$\cdot \left(\sum_d Q_x^{(1)}(l,d)\, x(d)\right)$$

$$\cdot \left(\sum_e Q_y^{(1)}(j,e)\, y(e)\right)$$

$$\cdot \left(\sum_f Q_z^{(0)}(k,f)\, y(f)\right)$$

$$\triangleq V_x(d,e)\, V_y(d,e)\, V_z(d,e)$$

Define $q_{ix}^{(0)T}$ to be the i^{th} row of $Q_x^{(0)}$. Then:

$V_x(d,e)$

$$= \left(\sum_a Q_x^{(1)}(i,a)\,x(a)\right)\cdot\left(\sum_d Q_x^{(1)}(l,d)\,x(d)\right)$$

$$= q_{ix}^{(1)T}x \cdot q_{lx}^{(1)T}x$$

$$= x^T\left(q_{ix}^{(1)}\;q_{lx}^{(1)T}\right)x$$

Let $S' = q_{ix}^{(1)}\;q_{lx}^{(1)T}$

Let
$$s = \begin{bmatrix} S'(1,1) \\ S'(1,2)+S'(2,1) \\ S'(1,3)+S'(2,2)+S'(3,1) \\ S'(1,4)+S'(2,3)+S'(3,2)+S'(1,4) \\ S'(2,4)+S'(3,3)+S'(4,2) \\ S'(3,4)+S'(4,3) \\ S'(4,4) \end{bmatrix}$$

And let

$$\underline{x} = \begin{bmatrix} 1 \\ x \\ x^2 \\ x^3 \\ x^4 \\ x^5 \\ x^6 \end{bmatrix} \qquad \underline{i} = \begin{bmatrix} 1 \\ 1/2 \\ 1/3 \\ 1/4 \\ 1/5 \\ 1/6 \\ 1/7 \end{bmatrix}$$

Then

$$V_x(d,e) = s^T \underline{x}$$

And

$$\int_0^1 V_x(d,e)\, dx = s^T \underline{i}$$

Therefore

$$\iiint V \, dx\, dy\, dz$$

$$= \int V_z \left(\int V_y \left(\int V_x \, dx \right) dy \right) dz$$

$$= s_x^T \underline{i} \cdot s_y^T \underline{i} \cdot s_z^T \underline{i} \,.$$

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