Variational Calculus and Discrete Alternatives

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The basic idea: instead of considering the change in a function wrt its arg, consider the variation in a functional wrt a variation in the function, this should be zero at the minimum of the functional.

The trick: if $\int f(x)q(x)dx = 0$ regardless of what q is, then f must be zero.

$y = f(x)$	definitions:
$F(y, y', x)$	function of the function, eval at a particular point, scalar
$q(x)$	test function added to f, zero at ends
$\delta f = (f + \epsilon q) - f = \epsilon q$	variation of function *at a particular point, scalar*
$E(F(f(x), f'(x), x))$ e.g. $E = \int f'(x)^2 dx$	functional maps function to scalar
$E[f] = \int F(y, y', x)dx$	general form of functional, maps function to scalar
	note E is function of f, not F
$\frac{\delta E}{\delta f} = 0 = \frac{dE}{d\epsilon}$ condition for minimum	functional does not change with small variation
$\delta \int f(x)dx = \int \delta f dx$	properties: variation commutes with integration, differentiation
$\delta F(y, y', x) = F(y + \epsilon q, y' + \epsilon q', x) - F(y, y', x)$	represent variation of function (not functional) by taylor exp
$= \frac{\partial F}{\partial y}\frac{dy}{d\epsilon}\delta\epsilon + \frac{\partial F}{\partial y'}\frac{dy'}{d\epsilon}\delta\epsilon + \frac{\partial F}{\partial x}\frac{dx}{d\epsilon}\delta\epsilon$	recognize 1. $dx/d\epsilon$ is zero, 2. ϵ is small, so say ϵ instead of $d\epsilon$
$= \epsilon\left(\frac{\partial F}{\partial y} q + \frac{\partial F}{\partial y'} q'\right)$	
	now look at variation of functional
$\delta E = \delta \int F dx = \int \delta F dx = \epsilon \int \left(\frac{\partial F}{\partial y} q + \frac{\partial F}{\partial y'} q'\right) dx$	divide by ϵ to get rate of change
$\frac{dE}{\epsilon} = \int \left(\frac{\partial F}{\partial y} q + \frac{\partial F}{\partial y'} q'\right) dx$	now do integration by parts on second term
$\int \frac{\partial F}{\partial y'} q' dx = \frac{\partial F}{\partial y'} q - \int \frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right) q dx$	: $\int ab' = ab - \int a'b$
$\left.\frac{\partial F}{\partial y'} q\right\|_b^a = 0$	because q is zero at both ends
$\frac{dE}{d\epsilon} = \int \left(\frac{\partial F}{\partial y} - \int \frac{d}{dx}\frac{\partial F}{\partial y'}\right) q dx$	and because q is arbitrary
$\frac{\partial F}{\partial y} - \frac{d}{dx}\frac{\partial F}{\partial y'} = 0$	euler-lagrange eqn

Worked Example: Laplace eqn in 1D

minimize $\int (f'(x))^2 dx$	should come out like $\frac{d^2 f}{dx^2} = \nabla^2 = 0$
$F(y, y', x) = y'^2$	
$\delta F = \frac{\partial F}{dy'}\frac{dy'}{d\epsilon}\delta\epsilon$	
$= \frac{\partial F}{dy'} q' \delta\epsilon$	$\frac{\partial F}{dy'} = 2y' = 2\frac{df}{dx}$
$\frac{dE}{d\epsilon} = \int \frac{\partial F}{dy'} q' dx$	now change q' to q
$\int \frac{\partial F}{dy'} q' dx = \frac{\partial F}{dy'} q - \int \frac{d}{dx}\frac{\partial F}{dy'} q dx$	integration by parts
$\left.\frac{\partial F}{dy'} q\right\|_a^b = 0$	because q is zero at both ends
$\frac{dE}{d\epsilon} = -\int \frac{d}{dx}\frac{\partial F}{dy'} q dx = 0$	variation of functional is zero at minimum
$= -2\frac{d}{dx}\frac{df}{dx} = -2\frac{d^2 f}{dx^2} = -2\nabla^2 f = 0$	

Dan Piponi's Physics Style approach to Variational Calculus

Need these:

δ is variation on the left, dirac on the right $\quad \dfrac{\delta u(z)}{\delta u(w)} = \delta(z - w)$

$$\frac{\delta \frac{d}{dx} u(z)}{\delta u(w)} = \frac{d}{dx}\delta(z - w)$$

true if a,b are zero at boundaries of integration $\quad \displaystyle\int a \frac{d}{dx} b = - \int \frac{da}{dx} b$

(this is like finite difference $aDb = -(Da)'b = -a'D'b$ which is true because if D = -1 1 ... then D' = 1 -1 ...)

chain rule $\quad \dfrac{\delta}{du(z)} f(u(x)) = f'(u(x)) \dfrac{\delta u(x)}{\delta u(z)}$

(' = derivative)

goal

$$\min \int (u')^2 dx$$

set first variational derivative to zero $\quad \displaystyle 0 = \frac{\delta}{\delta u(z)} \int u'(x)^2 dx$

$$= \int \frac{\delta}{\delta u(z)} u'(x)^2 dx$$

apply chain rule $\quad \displaystyle = \int 2u'(x) \frac{\delta u'(x)}{\delta u(z)} dx$

apply second relation above $\quad \displaystyle = \int 2u'(x) \frac{d}{dx} \delta(x - z) dx$

apply third relation above $\quad \displaystyle = \int -2 \frac{d}{dx} u'(x) \delta(x - z) dx$

integral and delta cancel each other, true at all z: $\quad \displaystyle = -2 \frac{d^2 u}{dx^2} = 0$

Ken Anjyo's approach

This approach starts directly with a general expression for the first variational derivative. (Setting this to zero is called "first order optimality condition" in the Chan&Wong paper).

Given a functional E that is an integral of a function $F(\vec{x}, u, u', u'', \ldots)$ of

- the coordinates $x_1, x_2, \ldots$,
- the unknown solution u
- and its nth order derivatives $u' = u_1, u'' = u_2$,

the general expression for the first variational derivative is:

$$\frac{\delta E}{\delta u} = F_u + \sum (-1)^n \frac{d^n}{dx^n} F_{u_n} = 0$$

(where the sum is over the order of derivative of u).

If $\frac{d^0}{dx^0}$ is read as identity this reduces to

$$\frac{\delta E}{\delta u} = \sum_0 (-1)^n \frac{d^n}{dx^n} F_{u_n} = 0$$

Apply this to the Laplace eqn: here n=1, $F(x, u, u', \ldots) = (u')^2$, $F_{u'} = 2u'$,

$$\frac{\delta E}{\delta u} = (-1)^n \frac{d}{dx} F_{u'} = -2 \frac{d}{dx} u' = -2 \frac{d^2}{dx^2} u = 0$$

See 2d application below

Discrete alternative 1

By considering the function as being a point in hilbert space, the functional is simply a function of an (infinite dimensional) point, so standard function minimization can be used.

Discrete alternative 2

From Lanczos book,

y_-, y, y_+	notation: y_{k-1}, y_k, y_{k+1}
$z = y' = (y_+ - y)/(x_+ - x)$	discrete derivative
$E = \sum F(y, z, x)(x_+ - x)$	
$\frac{dE}{dy_+} = \frac{d}{dy_+}[F(y, z, x)\Delta x] + \frac{d}{dy_+}\left[F(y_+, z_+, x_+)\Delta x\right]$	two terms in the sum involve y_+
$= \frac{d}{dy_+}A + \frac{d}{dy_+}B$	
$\frac{dA}{dy_+} = \frac{\partial F}{dy}\frac{dy}{dy_+}\Delta x + \frac{\partial F}{dz}\frac{dz}{dy_+}\Delta x + \frac{\partial F}{dx}\frac{dx}{dy_+}\Delta x$	$\frac{dx}{dy_+} = 0$, $\frac{dy}{dy_+} = 0$, $\frac{dz}{dy_+} = \frac{1}{\Delta x}$
$= \frac{\partial F}{dz}\frac{1}{\Delta x}\Delta x$	
$\frac{dB}{dy_+} = \frac{\partial F}{dy_+}\frac{dy_+}{dy_+}\Delta x + \frac{\partial F}{dz_+}\frac{dz_+}{dy_+}\Delta x + \frac{\partial F}{dx_+}\frac{dx_+}{dy_+}\Delta x$	$\frac{dx_+}{dy_+} = 0$, $\frac{dy_+}{dy_+} = 1$, $\frac{dz_+}{dy_+} = -\frac{1}{\Delta x}$
$= \frac{\partial F}{dy_+}\Delta x - \frac{\partial F}{dz_+}\frac{1}{\Delta x}\Delta x$	
total $= \frac{\partial F}{dy_+}\Delta x + \frac{\partial F}{dz} - \frac{\partial F}{dz_+}$	divide by Δx
$\frac{\partial F}{dy_+} - \frac{1}{\Delta x}\left(\frac{\partial F}{dz_+} - \frac{\partial F}{dz}\right)$	
$\frac{\partial F}{dy_+} = \Delta\left(\frac{1}{\Delta x}\frac{\partial F}{dy'}\right)$	as $\Delta x \to 0$ $\frac{\Delta}{\Delta x} \to \frac{d}{dx}$

Modified continuous

Take the Laplace eqn in 1D again, different derivation setup:

$E[f] = \int \left(\frac{df}{dx}\right)^2 dx$	(a) continuous
$E[f + \epsilon q] = \int \left((\frac{df}{dx})^2 + 2\frac{df}{dx}\epsilon q' + (\epsilon q)^2\right) dx = E[f] + 2\epsilon \int \frac{df}{dx} q' +$ Terms(q^2)	
$\delta E = E[f + \epsilon q] - E[f] = 2\epsilon \int \frac{df}{dx} q' dx$	
$\frac{dE}{d\epsilon} = 2\int \frac{df}{dx} q' dx$	get rid of q'
$\int \frac{df}{dx} q' dx = \frac{df}{dx} q \Big\vert - \int \frac{d}{dx}\frac{df}{dx} q dx$	integration by parts
$\frac{dE}{d\epsilon} = -2\int \frac{d}{dx}\frac{df}{dx} q dx$	for arbitrary q
$\frac{d}{dx}\frac{df}{dx} = \frac{d^2 f}{dx^2} = 0$	

Discrete alternatives 3,4

Is there a discrete equivalent to the variational calculus approach (which is: the functional is minimized then a variation of the function gives zero variation to the functional)?

Discrete 3

Now do something similar (to the modified continuous) discretely:

$E[f] = f' D' D f$	Df?
$\delta E = (f + \epsilon q)' D' D(f + \epsilon q) - f' D' D f$	discrete variation
$E[f + \epsilon q] = f' D' D f + 2 f' D' D \epsilon q +$ terms(ϵq^2)	(b') similar to continuous (b)
$\delta E = 2 f' D' D \epsilon q$	note this is a scalar
	want change in this wrt ϵq
$\frac{\partial E}{\partial \epsilon q} = 2 D' D f$	note this is a vector

$$D = \begin{bmatrix} 1 & & & \\ -1 & 1 & & \\ & -1 & 1 & \\ & & & \cdots \end{bmatrix}$$

$$D' = \begin{bmatrix} 1 & -1 & & \\ & 1 & -1 & \\ & & 1 & -1 \\ & & \cdots & \end{bmatrix}$$

D'D is 2 on the diagonal, -1 on the neighbors to diagonal, zero elsewhere, so -1 2 1 — this is $-\nabla^2$. The minus sign does not matter since the rhs is zero, but it comes out the same way as the continuous, both are negative. (Bishop appendix on variational calc talks about adjoint of derivative being the negative of the derivative).

Discrete 4

But easier to just directly minimize wrt f:

$$E[f] = f'D'Df \qquad \text{discrete}$$
$$dE/df = 2D'Df$$

TV deconvolution problem

Next apply these methods to the total variation blind deconvolution functional.

(Part of) that functional: $E = \int |\nabla u| = \int \sqrt{u_x^2 + u_y^2}$.

Apply the general solution expression (Ken Anjyo's approach):

- $\frac{\delta E}{\delta u} = F_u + \sum (-1)^n \frac{d}{d_x} F_{u_n} = 0$
- rewrite this for 2 dimensions, p==du/dx, q==du/dy, $p^n = d^n u/dx^n$.
- $F(x, y, u, p, q) = \sqrt{p^2 + q^2}$.
- $\frac{\delta E}{\delta u} = F_u + \sum (-1)^n \frac{d^n}{dx^n} F_{p^n} + \sum (-1)^n \frac{d^n}{dy^n} F_{q^n}$
- for TV problem $n = 1$, $F_u = 0$, $F_p = \frac{p}{\sqrt{p^2+q^2}}$, $F_q = \frac{q}{\sqrt{p^2+q^2}}$
- $\frac{\delta E}{\delta u} = -1 \frac{d}{dx} \frac{p}{\sqrt{p^2+q^2}} - 1 \frac{d}{dy} \frac{q}{\sqrt{p^2+q^2}} = -\frac{1}{\sqrt{p^2+q^2}} (\frac{d}{dx} p + \frac{d}{dy} q)$
- $= -\nabla \cdot \frac{\nabla u}{|\nabla u|}$

Variational version of Lagrange multiplier

With a constraint such as $\sum p_k = c$, the variational formulation of this constraint (to be added to some equation with a Lagrange multiplier) is: $\sum \delta p_k = 0$. This is derived like so:

$$\sum (p_k + \delta p_k) = c$$

$$\sum p_k + \sum \delta p_k = c$$

and then subtract the $\sum p_k$ and the c from this.