OPTIMALITY IN NUMERICAL DIFFERENTIATION

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1. INTRODUCTION

Consider the problem of estimating the mth derivative of a data function $g(x)$, given only N sampled values

$$y_n = g(x_n) + \varepsilon_n, \quad n = 0,\ldots, N-1, \tag{1}$$

where ε_n are uncorrelated random errors with mean zero and common variance σ^2 (possibly unknown). For simplicity consider equally-spaced sampling points $x_n = n/N$ on the interval $[0,1)$. Let m be a strictly positive integer, and denote the mth derivative by $f(x) = g^{(m)}(x)$, which is to be estimated on the interval $0 \leqslant x \leqslant 1$.

If K denotes an integral operator such that $Kf = g$, then a stabilized derivative can be constructed using pth-order Tikhonov regularization:

$$\min_{f \subset F_p} \left\{ \frac{1}{N} \sum_{n=0}^{N-1} [(Kf)x_n) - y_n]^2 + \lambda \|f\|_p^2 \right\}, \tag{2}$$

where F_p is a suitably chosen Hilbert space with norm $\|\cdot\|_p$ parametrized by the order of regularization $p > 0$, and the constant $\lambda \geqslant 0$ is the regularization parameter. Let $f_{N;\underset{\sim}{\alpha}}$ denote the minimizer of (2), where $\underset{\sim}{\alpha}$ is the parameter pair $\underset{\sim}{\alpha} = (p,\lambda)$.

In theory we may define an *absolutely optimal* parameter set $\underset{\sim}{\alpha}$ as that which minimizes (with respect to $\underset{\sim}{\alpha}$) the error

$$\|f_{N;\underset{\sim}{\alpha}} - f\|_F \tag{3}$$

where $\|.\|_F$ denotes the strongest norm consistent with the smoothness of the exact derivative f. In the data space there will exist a norm $\|.\|_G$ such that (3) and

$$\|Kf_{N;\underset{\sim}{\alpha}} - g\|_G \tag{4}$$