ON THE DISTRIBUTIONAL SOLUTION OF THE INVERSE PROBLEM INDUCED BY THE HEAT KERNEL METHOD

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As the first constrained step in the investigation of the Fokker-Planck equation as a source of the probability density function of the position (or velocity) of a Brownian particle, we studied the connection between the inverse problem for the diffusion equation and the kernel methods developed in the area of statistical learning theory and its applications.

The initial condition (an initial probability density function) is not known, and the solution of the diffusion equation (an output function) is presumed to be known at a finite, sufficiently large empirical set of points $\{(x_i, y_i)\}$—a sample.

With the use of Tikhonov's regularizing method, we reduced the problem to the minimization of the empirical functional in the *reproducing kernel Hilbert space H*:

$$R(\tilde{f}, \gamma) = \frac{1}{m}\sum_{i=1}^{m}\left[y_i - \tilde{f}(x_i)\right]^2 + \gamma\|\tilde{f}\|_H^2, \tag{1}$$

which led to the following formula for the approximate solution (the kernel function) of the diffusion problem:

$$\tilde{f}(x, t; \mathbf{c}) = \sum_{i=1}^{l} c_i K(x - x_i, t) \in H, \tag{2}$$

where $K(x,t)$ is the fundamental solution of the heat operator and the vector $\mathbf{c}$ of the coefficients is uniquely identified via regular linear algebra methods.

Such a formula can be applied in statistical analyses of the data generated by the physical model and in other tasks.

We discovered that there is no classical solution to the inverse problem that will generate the output in the form (2), but rather a distributional one. We proved the uniqueness of such solutions and provided physical/statistical motivation for this phenomenon.

The kernel functions we investigated at this stage of the project served as a first step toward the spectrum of physically motivated models involving multidimensional domains and equations with variable coefficients, noisy data, and so forth.

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