

From Kernel Regression to Attention Mechanisms: A Six Decade Journey (1960–2020)

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Abstract

This document outlines the conceptual evolution from classical kernel regression methods in statistics to the attention mechanisms foundational to modern machine learning. It traces a path through three major periods: Kernel Regression (1960s–1990s), Data-Adaptive Filters in signal processing (1990s–2010s), and Attention Mechanisms in machine learning (2010s–2020s) [1].

1 Kernel Regression (Nadaraya-Watson, 1964)

The journey begins with kernel regression, a non-parametric method to fit a smooth curve to data points by modeling a nonlinear relationship [2]. At any query position x , the value $\hat{y}(x)$ is estimated as a weighted average of observed data y_i . The weights are determined by a kernel function, $K(x, x_i)$, which measures the proximity between the query point x and each data point x_i . The Nadaraya-Watson estimator is given by:

$$\hat{y}(x) = \frac{\sum_i K(x, x_i) y_i}{\sum_i K(x, x_i)} \quad (1)$$

A common choice for the kernel is the Gaussian (or Radial Basis Function) kernel:

$$K(x_i, x_j) = \exp \left\{ \frac{-\|x_i - x_j\|^2}{h_x^2} \right\} \quad (2)$$

where h_x is a bandwidth parameter controlling smoothness.

2 Evolution in Signal Processing: Data-Adaptive Filters

The concepts from kernel regression were extended in signal and image processing to create powerful data-adaptive filters. These filters generalize the kernel to consider not just spatial distance but also similarity in data values (e.g., pixel intensities).

2.1 Bilateral Filter (Tomasi & Manduchi, 1998)

The Bilateral Filter extends the kernel to operate on both the positions (domain) and the values (range) of pixels, allowing it to smooth images while preserving sharp edges [3]. The kernel includes a term for value similarity:

$$K(x_i, x_j, y_i, y_j) = \exp \left\{ \frac{-\|x_i - x_j\|^2}{h_x^2} - \frac{(y_i - y_j)^2}{h_y^2} \right\} \quad (3)$$

2.2 Non-local Means (Buades, Coll, & Morel, 2005)

Non-local Means further generalizes this idea by comparing entire patches of pixels rather than individual pixel values, making it more robust to noise [4]. The kernel is defined as:

$$K(x_i, x_j, \mathbf{p}_i, \mathbf{p}_j) = \exp \left\{ \frac{-\|x_i - x_j\|^2}{h_x^2} - \frac{\|\mathbf{p}_i - \mathbf{p}_j\|^2}{h_y^2} \right\} \quad (4)$$

where \mathbf{p}_i and \mathbf{p}_j represent the image patches centered at positions x_i and x_j .

2.3 Locally Adaptive Regression Kernel (LARK)

LARK, developed by Takeda et al. [5] and related to the work of Sochen et al. [6], introduced a "Learned Metric" where the kernel's shape adapts to the local data structure:

$$K(x_i, x_j, y) = \exp \left\{ -(x_i - x_j)^T \mathbf{C}_{ij}(y) (x_i - x_j) \right\} \quad (5)$$

Here, $\mathbf{C}_{ij}(y)$ is a matrix capturing the local data geometry.

3 A Unified Framework

These methods can be viewed under a single framework by defining an augmented variable t combining position and value information. The generalized kernel is written in a quadratic form:

$$K(t_i, t_j) = \exp \left\{ -(t_i - t_j)^T \mathbf{Q}_{i,j} (t_i - t_j) \right\} \quad (6)$$

where \mathbf{Q} is a block matrix $\mathbf{Q} = \text{diag}(\mathbf{Q}_x, \mathbf{Q}_y)$ that changes form for each method. This unified perspective is detailed in Milanfar (2013) [7].

4 From Kernels to Attention Mechanisms

The final leap in this evolution is the attention mechanism, which can be seen as a learned, generalized form of the Nadaraya-Watson estimator [1]. The core components are vectors representing a **Query** (Q), a **Key** (K), and a **Value** (V).

The mechanism computes an output for each query by taking a weighted sum of all values. The weights are derived from a compatibility function, or similarity score, between the query and each key. The structure illustrated in the presentation is a direct parallel to the kernel regression formula (1). The output \hat{y}_i for a given query q_i is computed as a normalized weighted sum over all values v_j :

$$\hat{y}_i = \frac{\sum_j \exp(\text{score}(q_i, k_j)) \cdot v_j}{\sum_j \exp(\text{score}(q_i, k_j))} \quad (7)$$

This is the structure of the softmax function applied to the raw similarity scores. Here, the kernel $K(x, x_i)$ from Equation (1) is effectively replaced by a learned similarity function passed through an exponential, $\exp(\text{score}(q_i, k_j))$. In modern architectures like the Transformer, this score is typically the scaled dot-product: $\text{score}(q_i, k_j) = q_i^T k_j / \sqrt{d_k}$. The query, key, and value vectors are themselves learned projections of input data, allowing the model to dynamically "attend" to the most relevant information.

References

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