Regression with Sparse Approximations of Data

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Regression with Sparse Approximations of Data
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Introduction

We propose SPARse appROximation WEighted regression (SPARROW), a new method for locally polynomial regression function estimation, and an extension of sparse representation classification to the regression setting.

To estimate the regression function at a point, SPARROW uses Taylor polynomial expansion around that point, least-squares optimal parameter estimation, and sparse approximation in terms of a dictionary of regressors and regressands.

Our results show that locally constant SPARROW performs competitively, but the locally linear form, with and without regularization, does not.

What is Local Regression?

Consider we have a dataset of N observations indexed by Ω := {1, ..., N}:

\[ D := \{(x_i, y_i) : x_i \in \mathbb{R}^d, y_i \in \mathbb{R}, i \in \Omega\} \]

We wish to estimate the regression function \( f(x) : \mathbb{R}^d \to \mathbb{R} \) at a point \( z \in \mathbb{R}^d \).

1. Approximating this function by a Taylor polynomial about \( z \), we have

\[ f(x) \approx f(z) + (x - z)^\top \theta_z + \frac{1}{2!}(x - z)^\top \theta_{zz}(x - z) \]

where \( \theta_z \) and \( \theta_{zz} \) are the gradient and Hessian of \( f(x) \), evaluated at \( z \).

2. We can solve for \( f(z), \theta_z \) and \( \theta_{zz} \) by

\[ \min_{f(z), \theta_z, \theta_{zz}} \sum_{i \in \Omega} \alpha_i(z) \left| y_i - \left( f(z) - (x_i - z)^\top \theta_z + \frac{1}{2}(x_i - z)^\top \theta_{zz}(x_i - z) \right) \right|^2 \]

where \( \alpha_i(z) \) is the \( i \)th observation weight. We can pose this as

\[ \min_{\Theta_z} \| A_z^\top (y - X_z \Theta_z) \|_2^2 \]

where \( A_z \) is an orthonormal basis of \( X_z \) and zero else, \( \Theta_z := (f(z), \theta_z, \text{vech}(\theta_{zz})) \), and \( X_z := \begin{bmatrix} 1 & (x_1 - z)^\top \text{vech}(z - x_1 - z)^\top \end{bmatrix}, \quad \begin{bmatrix} 1 & (x_2 - z)^\top \text{vech}(z - x_2 - z)^\top \end{bmatrix} \).

The notation vech(\( B \)) is the supervec of half of the symmetric matrix \( B \).

3. The first element of the solution \( \hat{\Theta}_z = (X_z^\top A_z X_z)^{-1} X_z^\top A_z y \) gives the least-squares optimal locally polynomial estimate of \( f(z) \)

\[ \hat{f}(z) = \begin{bmatrix} 1 & (x_1 - z)^\top \text{vech}(z - x_1 - z)^\top \end{bmatrix} \]

Taking only the first column of \( X_z \) gives a locally constant estimate of \( f(z) \):

\[ \hat{f}(z) = (1^\top A_z 1)^{-1} 1^\top A_z y = \sum_{i \in \Omega} \alpha_i(z) y_i \sum_{i \in \Omega} \alpha_i(z) \]

Taking the first two columns gives a locally linear estimate of \( f(z) \).

We must now define the \( N \) observation weights \( \{\alpha_i(z) : i \in \Omega\} \).

Weighted \( k \)-nearest neighbor regression (Wa-NNR) defines the weights by the reciprocal of their Euclidean distance to \( z \).

Nadaraya-Watson kernel regression (NWR) method defines the weights using a kernel function, e.g., Gaussian, evaluated with respect to \( z \).

SPARROW defines the weights using the sparse approximation of \( z \) with respect to the observed points in \( D \).

How SPARROW Defines the Observation Weights

We construct a dictionary matrix by concatenating normalized regressors

\[ D := \begin{bmatrix} x_1 & x_2 & \cdots & x_M \end{bmatrix} \]

For a given point \( z \), SPARROW finds a solution to \( z \approx D s \) such that \( s \) has many zero elements by solving the basis pursuit denoising (BPDN) problem

\[ \min_{s \in \mathbb{R}^M} \| s \|_1 \text{ subject to } \frac{\| z - D s \|_2}{\| z \|_2} \leq \epsilon^2 \]

where \( \epsilon^2 > 0 \). Defining \( \Sigma \) as a diagonal matrix of the unbiased estimates of the variances observed in the dimensions of the regressors in \( D \), SPARROW then defines the \( i \)th observation weight by

\[ s_i(z) := \frac{(z - x_i)^\top \Sigma^{-1}(z - x_i)}{\min_{x \in D} (z - x)^\top \Sigma^{-1}(z - x)} \]

Experiments and Simulations

<table>
<thead>
<tr>
<th>Dataset</th>
<th># observations (N)</th>
<th># attributes (M)</th>
<th>k</th>
</tr>
</thead>
<tbody>
<tr>
<td>Abalone</td>
<td>4,177</td>
<td>8</td>
<td>9</td>
</tr>
<tr>
<td>Bodyfat</td>
<td>252</td>
<td>14</td>
<td>4</td>
</tr>
<tr>
<td>Housing</td>
<td>506</td>
<td>13</td>
<td>2</td>
</tr>
<tr>
<td>MPG</td>
<td>392</td>
<td>7</td>
<td>4</td>
</tr>
</tbody>
</table>

Our test datasets are described in the table above, with the last column showing the tuned parameter \( k \) in our experiments with k-NNR and Wa-NNR. The figures below compare locally-constant SPARROW (C-SPAR) and other methods. We use 100 independent trials of 10-fold cross-validation to estimate the mean squared error (MSE). Red lines mark median. Boxes delimit 25 to 75 percentiles. Extrema marked by whiskers, and outliers by pluses.

For locally linear SPARROW (L-SPAR), we can employ regularization to solve

\[ \min_{\Theta_z, \lambda} \| A_z^\top (y - X_z \Theta_z) \|_2^2 + \lambda \| \Theta_z \|_2^2 \]

For the same datasets as above, the table below compares C-SPAR with L-SPAR with and without regularization. To estimate the MSE, we run 10 independent trials of 10-fold cross-validation. The last column denotes the ridge parameter to obtain the L-SPAR w/ \( R \) estimate.

<table>
<thead>
<tr>
<th>Dataset</th>
<th>C-SPAR</th>
<th>L-SPAR w/ R.</th>
<th>L-SPAR</th>
<th>( \lambda )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Abalone</td>
<td>5</td>
<td>16</td>
<td>988</td>
<td>10^{-3}</td>
</tr>
<tr>
<td>Bodyfat</td>
<td>5 \times 10^{-5}</td>
<td>35 \times 10^{-5}</td>
<td>960 \times 10^{-5}</td>
<td>10^{-6}</td>
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<tr>
<td>Housing</td>
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<td>45</td>
<td>4304</td>
<td>10^{-3}</td>
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<tr>
<td>MPG</td>
<td>7</td>
<td>8</td>
<td>6335</td>
<td>10^{-3}</td>
</tr>
</tbody>
</table>

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