Statistical Gradient Boosting of Generalised Additive Model with Ridge Regression on GPU

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Outline

Generalised Additive Model

The Gaussian Generalised Additive Model (GAM) is defined as:

$$\boldsymbol{y} \sim \mathcal{N}(\boldsymbol{\mu}, \sigma^2)$$
$$\boldsymbol{\mu} = \beta_0 + f_1(\boldsymbol{x}_1) + \ldots + f_p(\boldsymbol{x}_p)$$

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For an unknown $f(x_j)$, it is usually sensible to assume it's a smooth function, which can be represented as a linear combination of rank-reduced k basis functions $b_i(.)$ multiplied by their fitted coefficients γ_i:

$$f(\boldsymbol{x}_j) = \sum_{i=1}^{k} b_i(\boldsymbol{x}_j)\gamma_i = \mathbf{B}_j\boldsymbol{\gamma}_j$$

GAM – smooth functions

In order to enforce smoothness on $f_j(\boldsymbol{x}_j)$, the term $\lambda_j \boldsymbol{\gamma}_j^T \mathbf{S}_j \boldsymbol{\gamma}_j$ is typically added to the f_j's loss function, where $\mathbf{S}_j$ is the smoothing matrix and λ_j is the penalty term.

$$L = ||\boldsymbol{y} - \hat{\boldsymbol{\mu}}||^2 + \sum_{j=1}^{p} \lambda_j \boldsymbol{\gamma}_j^T \mathbf{S}_j \boldsymbol{\gamma}_j$$

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In our case we have chosen $\mathbf{S} = \mathbf{I}$, which results in a simple ridge penalty $\lambda_j ||\boldsymbol{\gamma}_j||^2$. However, there are many other, more complex penalties to choose from. For example, a P-Spline smooths the function by setting $\mathbf{S} = \mathbf{D}^T \mathbf{D}$, which enforces smoothness by penalising the changes in differences of adjacent coefficients:

$$\boldsymbol{\gamma}^T \mathbf{S} \boldsymbol{\gamma} = \sum_{i+1}^{k-1} (\gamma_{i-1} - 2\gamma_i + \gamma_{i+1})^2$$

Gradient Boosting

- Gradient boosting is a fitting algorithm, which sequentially fits weak estimators (a.k.a. base learners) to the gradient of the loss function $\mathbf{g}^{[m]}$.
- The resulting model can avoid including unnecessary base learners and shrink estimates from the included ones to reduce the generalisation error of the model.
- In GAMs, the base learners are typically penalised regression models – each with a design matrix $\mathbf{B}_j$, smoothing matrix $\mathbf{S}_j$, and the smoothing parameter λ_j.

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Smooth functions as base learners

At each iteration m, all K base learners are fitted to the residuals of the model $\mathbf{g}^{[m]}$:

$$\boldsymbol{\gamma}_j^{[m]} = (\mathbf{B}_j^T \mathbf{B}_j + \lambda_j \mathbf{S}_j)^{-1} \mathbf{B}_j^T \mathbf{g}^{[m]}$$

and the one with the lowest residual sum of squares is selected.

$$\text{learner index} = \arg\min_j ||\mathbf{g}^{[m]} - \mathbf{B}_j \boldsymbol{\gamma}_j^{(m)}||^2$$

The smoothing parameter λ_j is selected before the fitting process, such that the learner has some small number of effective degrees of freedom trace$(\mathbf{H}_j)$.

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Computational considerations

In gradient boosting, finding λ for each learner and the associated $(\mathbf{B}^T\mathbf{B} + \lambda\mathbf{S})^{-1}$ is relatively inexpensive as it can be done just once.

Operations that happen at each boosting iteration m are the main computational bottleneck and include the following matrix-vector multiplications:

1. $\mathbf{B}^T\mathbf{g}^{[m]}$, $O(np)$
2. $(\mathbf{B}^T\mathbf{B} + \lambda\mathbf{S})^{-1}(\mathbf{B}^T\mathbf{g}^{[m]})$, $O(p^2)$
3. $\mathbf{B}\boldsymbol{\gamma}^{[m]}$, $O(np)$

These can be sped up significantly by parallel computing.

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B-Splines as Base Learners

Matrix Vector Multiplication

Algorithm Naive Implementation of Matrix Vector Multiplication

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for i = 1 to M do
    y[i] ← 0
    for j = 1 to N do
        y[i] += A[i][j] * x[j]
    end for
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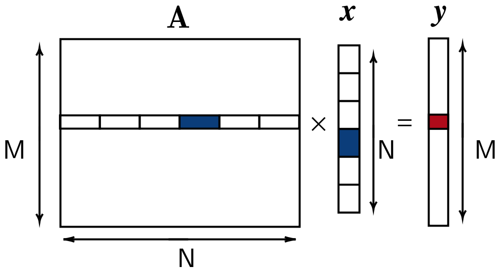
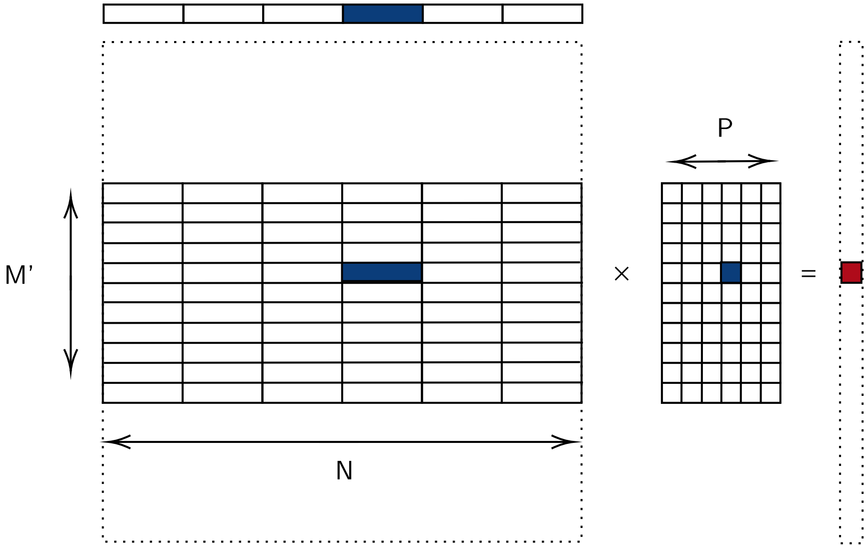
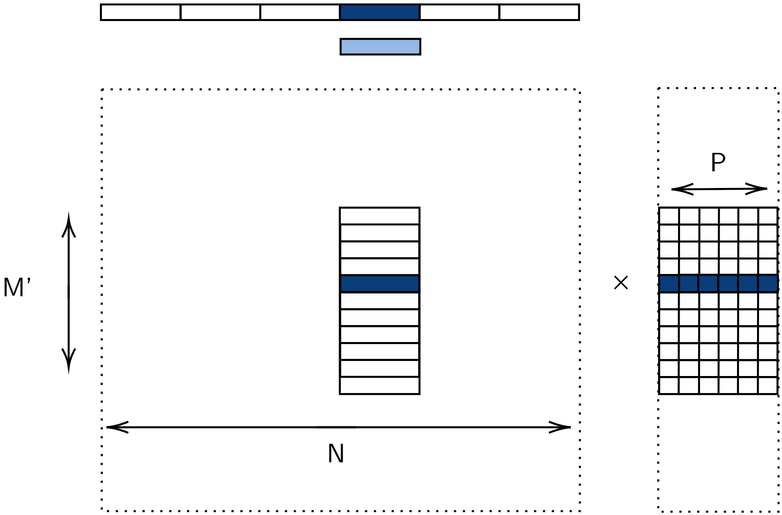


Parallelisation



Preloading of $\boldsymbol{x}_i$



Simulation

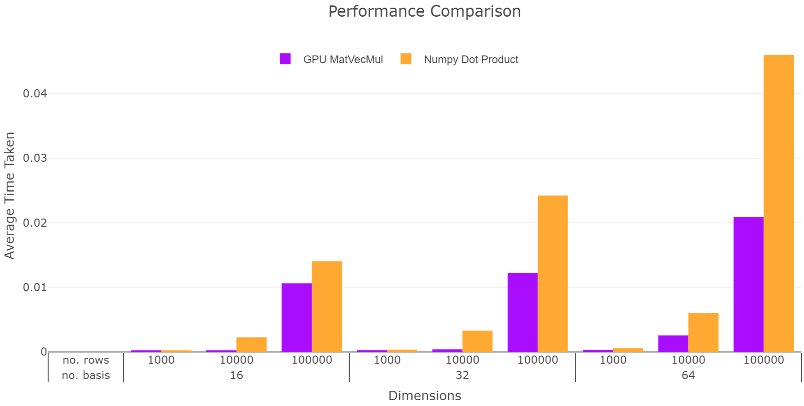


Figure: Comparison of Matrix Vector Multiplication between GPU and Numpy (CPU)

Reference

- Wang, Hansheng, and Chih-Ling Tsai. "*Tail index regression*." Journal of the American Statistical Association 104.487 (2009): 1233-1240.

Decomposing smooth functions

The basis matrix $\mathbf{B}$ can be reparametrised as a sum of smooth and unpenalised components:

$$\mathbf{B}\boldsymbol{\gamma} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{b}$$
$$\boldsymbol{\gamma}^T \mathbf{S}\boldsymbol{\gamma} = \mathbf{b}^T \mathbf{I}\mathbf{b}$$

which means we can split functions $f_j(\boldsymbol{x}_j)$ into separate base learners for unpenalised $(\mathbf{X}\boldsymbol{\beta})$ and smooth components $(\mathbf{Z}\mathbf{b})$.
This allows $f_j(\boldsymbol{x}_j)$ to take the form of a linear or smooth function independently of the other improving model interpretability and performance.