Gradient and Newton Boosting for Classification and Regression

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Abstract

Boosting algorithms show high predictive accuracy on a wide array of datasets. To date, the distinction between boosting with either gradient descent or second-order updates is often not made, and it is thus implicitly assumed that the difference is irrelevant. In this article, we present gradient and Newton boosting, as well as a hybrid variant of the two, in a unified framework. We compare these boosting algorithms with trees as base learners on a large set of regression and classification datasets using various choices of loss functions. Our experiments show that Newton boosting outperforms gradient and hybrid gradient-Newton boosting in terms of predictive accuracy on the majority of datasets. Further, we present empirical evidence that this difference in predictive accuracy is not primarily due to faster convergence of Newton boosting, but rather since Newton boosting often achieves lower test errors while at the same time having lower training losses. In addition, we introduce a novel tuning parameter for tree-based Newton boosting which is interpretable and important for predictive accuracy.

Keywords: Statistical boosting, supervised learning, ensembles, trees, prediction

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1 Introduction

Boosting refers to a type of classification and regression algorithms that enjoy large popularity due to their high predictive accuracy observed for a wide range of datasets [Chen and Guestrin, 2016]. The first boosting algorithms for classification, including the well known AdaBoost algorithm, were introduced by Schapire [1990], Freund and Schapire [1995], and Freund et al. [1996]. Later, several authors [Breiman, 1998, 1999, Friedman et al., 2000, Mason et al. 2000, Friedman, 2001] introduced the statistical view of boosting as a stage-wise optimization approach. See Schapire [2003], Bühlmann and Hothorn [2007], Schapire and Freund [2012], Mayr et al. [2014a], and Mayr et al. [2014b] for reviews on boosting algorithms in both the machine learning and statistical literature.

There exist broadly speaking two different approaches of statistical boosting for iteratively finding a minimizer in a function space: one that uses stagewise first-order functional gradient descent updates and one that is based on second-order functional Newton-Raphson updates. We denote these two approaches by gradient boosting and Newton boosting. In addition, one can combine gradient with Newton updates by learning a part of the parameters with a gradient step and the remaining parameters with a Newton step. In particular, if trees are used as base learners, one can learn the structure of the trees using a gradient step and update the leaves using Newton’s method. This approach is denoted by hybrid gradient-Newton boosting in the following. For more information, see Section 2 where we present these three types of boosting algorithms in a unified framework.

In both research and applied data analysis, the distinction between gradient and Newton boosting is often not made, and it is thereby implicitly assumed that the difference is not important. For instance, the two recent popular boosting libraries LightGBM and TF Boosted Trees do not distinguish in their companion articles [Ke et al., 2017, Ponomareva et al., 2017] between gradient and Newton boosting, and one has to assume that gradient boosting with potentially Newton updates for tree leaves is used. Further, Prokhorenkova et al. [2018] briefly mention in their article on CatBoost that the minimization for finding a boosting update can be done using the Newton method or with a gradient step, and then continue to write that “both methods are kinds of functional gradient descent”. However, Newton’s method is clearly different from gradient descent. Another example is Biau et al. [2018] in which an interesting extension of gradient boosting is introduce by adding Nesterov acceleration to the gradient step. However, Newton boosting, which also allows for faster
learning in the cases where it is applicable, is not mentioned.

In our empirical analysis, we find that Newton boosting often has lower test errors than both gradient boosting and hybrid gradient-Newton boosting with trees as base learners. Further, we observe that hybrid gradient-Newton boosting often has better predictive accuracy than gradient boosting. Interestingly, we also find that Newton boosting results in both lower in-sample training losses, which are essentially zero for most classification datasets, as well as lower out-of-sample test errors for most datasets.

To the best of our knowledge, a systematic comparison concerning the predictive accuracy of gradient, Newton, and hybrid gradient-Newton boosting for various choices of loss functions and regression and classification tasks has not been done so far. The $L_K$-TreeBoost algorithm of Friedman [2001] is compared in Friedman [2001] with $K$-class LogitBoost of Friedman et al. [2000] for classification with five classes in a simulation study for one type of random functions. In our terminology, $L_K$-TreeBoost is a version of hybrid gradient-Newton boosting and $K$-class LogitBoost corresponds to Newton boosting for the Bernoulli likelihood. Friedman [2001] finds that the algorithms perform “nearly the same” with “LogitBoost perhaps having a slight advantage”. In addition, it is mentioned that “it is likely that when the shrinkage parameter is carefully tuned for each of the three methods [$L_K$-TreeBoost, $K$-class LogitBoost, AdaBoost], there would be little performance differential between them.” Our empirical evidence is not in line with this statement. Saberian et al. [2011] also briefly compare variants of boosting with gradient and second-order updates using three different binary classification datasets and Haar wavelets as base learners. However, their boosting approach is different from ours, and also the one usually adopted in practice and research, in the sense that they assume normed based learners, find base learners as maxima of inner products of gradients and base learners, and perform an additional line search to find the step size. Further, tuning parameters such as the learning rate and the number of boosting iterations are not chosen using cross-validation, and only 25 boosting iterations are performed. In addition, no uncertainty in predictive accuracy is documented and no tests are done to investigate whether the differences are statistically significant. Nonetheless, they come to the same conclusion as we do, i.e., they find that their version of second-order boosting performs better than gradient boosting. The closest to our analysis is Li [2010]. He compares Newton boosting (“logitboost”) with hybrid gradient-Newton boosting (“mart”) for several multi-class classification datasets and also
finds that Newton results in lower test errors than hybrid gradient-Newton boosting. However, [Li 2010] only considers one sample split per dataset and thus ignores uncertainty in predictive accuracy, and tuning parameters are not chosen using cross-validation. Finally, [Sun et al. 2014] compare Newton and gradient boosting for binary classification using the logistic loss. Their focus is on the convergence rate and their empirical comparison only considers the training error, though.

In summary, the novel contributions of this article are the following ones. First, we show how gradient, Newton, as well as hybrid gradient-Newton boosting can be derived in a unified framework. In addition, we introduce a novel tuning parameter for Newton boosting with trees as base learners. We argue that this equivalent number of weighted samples per leaf parameter is a natural and interpretable tuning parameter which is important for predictive accuracy. Further, we are the first to systematically compare gradient, Newton, and hybrid gradient-Newton boosting on a large set of both real-world and simulated classification and regression datasets.

2 The statistical view of boosting: three approaches for stagewise optimization

In this section, we present the statistical view of boosting as finding the minimizer of a risk functional in a function space using a stagewise, or greedy, optimization approach. We distinguish between gradient and Newton boosting as well as a hybrid version of the two and show how these can be presented in a unified framework. Note that these boosting algorithms have been proposed in prior research [e.g., Breiman 1998, 1999, Friedman et al. 2000, Mason et al. 2000, Friedman 2001, Saberian et al. 2011], but, to the best of our knowledge, the presentation below in a unified framework and the extension to the multivariate case is novel.

We note that, originally, boosting and, in particular, AdaBoost was motivated differently from the currently adopted statistical view of boosting as a stagewise optimization procedure. Although there is some debate on whether the statistical view of boosting helps to understand the success of AdaBoost [Mease and Wyner 2008, Wyner et al. 2017], we focus on statistical boosting in this article mainly because it provides a unified framework which allows for generalizing boosting to the regression setting or any other suitable loss
function.

2.1 Population versions

We assume that there is a response variable \( Y \in \mathbb{R} \) and a vector of predictor variables \( X \in \mathbb{R}^p \). Our goal is to predict the response variable using the predictor variables, where predictions can be done both deterministically or probabilistically. We assume that \( (Y, X) \) are random variables on \( \mathbb{R} \times \mathbb{R}^p \) where both the distribution of \( X \) and the conditional distribution \( Y|X \) are absolutely continuous with respect to either the Lebesgue measure, a counting measure, a mixture of both, or a product measure of the former measures. In particular, this covers both regression and classification tasks or mixtures of the two such as Tobit regression [see, e.g. Sigrist and Hirnschall 2017].

The goal of boosting is to find a minimizer \( F^* \) of the risk \( R(F) \) which is defined as the expected loss

\[
R(F) = E_{Y,X}(L(Y,F(X))),
\]

where \( F(\cdot) \) is a function in a Hilbert space \( \mathcal{H} \) with inner product \( \langle \cdot, \cdot \rangle \) given by

\[
\langle F, F \rangle = E_X (F(X)^2),
\]

and \( L(Y,F) \) is an appropriately chosen loss function. See below and Appendix A for examples of loss functions. Note that for notational simplicity, we often denote a function \( F(\cdot) \) shortly by \( F \) in this article. In general, the \( F \) can also be a multivariate function in a direct sum Hilbert space. For notational simplicity, we assume in the following that \( F \) is univariate. In Section 2.3 we extend this to the multivariate case.

Boosting assumes that the minimizer \( F^* \) lies in the span of a set of so-called base learners. I.e., \( F^* \in \Omega_S \), where \( \Omega_S = \text{span}(S) \) and \( S \) is a set of base learners \( f_j : \mathbb{R}^p \to \mathbb{R} \):

\[
F^* = \arg\min_{F \in \Omega_S} R(F).
\]

If the risk \( R(F) \) is convex in \( F \), then (2) is a convex optimization problem since \( \Omega_S \) is also convex.

\footnote{For the sake of simplicity, we focus on univariate \( Y \in \mathbb{R} \). The extension to the case of a multivariate response variable \( Y \) is straightforward. See also Section 2.3 where we present multivariate versions of boosting.}
Boosting finds $F^*$ in a stagewise way by sequentially adding an update $f_m$ to the current estimate $F_{m-1}$,

$$F_m(x) = F_{m-1}(x) + f_m(x), \quad f_m \in S, \quad m = 1, \ldots, M,$$

such that the risk is minimized

$$f_m = \arg\min_{f \in S} R (F_{m-1} + f).$$

This minimization can often not be done analytically and, consequently, an approximation has to be used.

Different boosting algorithms vary in the way the minimization in (4) is done, the loss function $L$ used in (1), and in the choice of base learners $f_j \in S$. Concerning loss functions, potential choices include the squared loss $L(y, F) = (y - F)^2 / 2$ for regression, the negative Gaussian log-likelihood where both the mean and the scale parameter depend on predictor variables [see, e.g., Mayr et al., 2012], the negative log-likelihood $-yF + \log (1 + e^F)$ of a binomial model with a logistic link function for binary classification, or the entropy loss with a softmax function for multiclass classification. Under appropriate regularity assumptions, one can use the negative log-likelihood of any statistical model as loss function:

$$L(y, F) = -\log (f_{F,\theta}(y)),$$

where $f_{F,\theta}(y)$ is the density of $Y$ given $X$ with respect to some reference measure, $F$ is linked to one or several, possibly transformed, parameters of this density and $\theta$ are additional parameters. See Appendix A for various examples of loss functions and, in particular, the ones we consider in the empirical evaluation of this article.

Concerning base learners, regression trees [see, e.g., Breiman et al., 1984] are the most frequently used choice. Other potential base learners include splines or linear functions [Bühlmann and Yu, 2003, Bühlmann et al., 2006, Schmid and Hothorn, 2008]. In this article, we focus on trees:

$$f(x) = w_s(x),$$

where $s : \mathbb{R}^p \to \{1, \ldots, J\}, \ w \in \mathbb{R}^J, \text{ and } J \in \mathbb{N}$ denotes the number of terminal nodes, or leaves, of the tree $f(x)$. The function $s$ represents the structure of the tree, i.e., the partition of the space $\mathbb{R}^p$, and $w$ contains the values of the leaves. As in Breiman et al. [1984], we assume that the partition of the space made by $s$ is a binary tree where each
cell in the partition is a rectangle of the form $R_j = (l_1, u_1] \times \cdots \times (l_p, u_p] \subset \mathbb{R}^p$ with $-\infty \leq l_m < u_m \leq \infty$ and $s(x) = j$ if $x \in R_j$.

For finding an update in (3), either a form of gradient descent, the Newton method, or a hybrid variant is used to obtain an approximate solution to the minimization problem in (4). In the following, we describe these approaches.

2.1.1 Gradient boosting

Assuming that $R(F)$ is Gâteau differentiable for all $F \in \Omega_S$, we denote the Gâteau derivative by

$$dR(F, f) = \frac{d}{d\epsilon} R(F + \epsilon f) \bigg|_{\epsilon=0} = \lim_{\epsilon \to 0} \frac{R(F + \epsilon f) - R(F)}{\epsilon}, \quad F, f \in \Omega_S.$$ 

Gradient boosting then works by choosing $f_m$ as the minimizer of a first order Taylor approximation with a penalty on the norm of the base learner:

$$f_m = \arg\min_{f \in S} R(F_{m-1}) + dR(F_{m-1}, f) + \frac{1}{2} \langle f, f \rangle$$

$$= \arg\min_{f \in S} dR(F_{m-1}, f) + \frac{1}{2} \langle f, f \rangle.$$ 

(5)

Note that we add the penalty $\frac{1}{2} \langle f, f \rangle$ since the functions $f$ are not necessarily normed and $\langle f, f \rangle$ is not assumed to be constant.

If we assume that $L(Y, F)$ is differentiable in $F$ for P-almost all $X$ and that this derivative is integrable with respect to the measure of $(Y, X)$, then $dR(F_{m-1}, f)$ is given by

$$dR(F_{m-1}, f) = E_{Y,X} (g_m(Y, X)f(X)),$$

where $g_m(Y, X)$ denotes the gradient of the loss function $L(Y, F)$ with respect to $F$ at the current estimate $F_{m-1}$:

$$g_m(Y, X) = \frac{\partial}{\partial F} L(Y, F) \bigg|_{F=F_{m-1}(X)}.$$  

(6)

Consequently, (5) can be written as

$$f_m = \arg\min_{f \in S} E_{Y,X} \left( g_m(Y, X)f(X) + \frac{1}{2} f(X)^2 \right)$$

$$= \arg\min_{f \in S} E_{Y,X} \left( (-g_m(Y, X) - f(X))^2 \right).$$  

(7)

This shows that $f_m$ is the $L^2$ approximation to the negative gradient $-g_m(Y, X)$ of the loss function $L(Y, F)$ with respect to $F$ evaluated at the current estimate $F_{m-1}(X)$. 


If the following expression is well defined for P-almost all $X$, then the minimization in (7) can also be done pointwise:

$$f_m(X) = \arg\min_{f \in S} E_{Y|X} \left( (-g_m(Y,X) - f(X))^2 \right).$$

### 2.1.2 Newton boosting

For Newton boosting, we assume that $R(F)$ is two times Gâteau differentiable and denote the second Gâteau derivative by

$$d^2 R(F,f) = \left. \frac{d^2}{d\epsilon^2} R(F + \epsilon f) \right|_{\epsilon=0}, \quad F, f \in \Omega_S.$$

Newton boosting chooses $f_m$ as the minimizer of a second order Taylor approximation

$$f_m = \arg\min_{f \in S} R(F_m - 1) + dR(F_m - 1, f) + \frac{1}{2} d^2 R(F_m - 1, f). \quad (8)$$

If we assume the P-almost all existence and integrability of the second derivative of $L(Y,F)$ with respect to $F$, then (8) can be written as

$$f_m = \arg\min_{f \in S} E_{Y,X} \left( g_m(Y,X)f(X) + \frac{1}{2} h_m(Y,X)f(X)^2 \right) \quad (9)$$

where the gradient $g_m(Y,X)$ is defined in (6) and $h_m(Y,X)$ is the Hessian of $L(Y,F)$ with respect to $F$ at $F_m - 1$:

$$h_m(Y,X) = \left. \frac{\partial^2}{\partial F^2} L(Y,F) \right|_{F=F_m-1(X)}. \quad (10)$$

The last line in Equation (9) shows that $f_m$ is the weighted $L^2$ approximation to negative ratio of the gradient over the Hessian $-\frac{g_m(Y,X)}{h_m(Y,X)}$ where the weights are given by the second derivative $h_m(Y,X)$.

If the following expression is well defined for P-almost all $X$, we can again calculate the pointwise minimizer of (9) as:

$$f_m(X) = \arg\min_{f \in S} E_{Y|X} \left( h_m(Y,X) \left( -\frac{g_m(Y,X)}{h_m(Y,X)} - f(X) \right)^2 \right).$$

Note that gradient boosting can be seen as a special case of Newton boosting. If the second derivative of the loss function $h_m(Y,X)$ exists and is constant, $h_m(Y,X) = c \in \mathbb{R}\setminus\{0\}$, for P-almost all $X$, then the Newton boosting update in (9) essentially equals the
gradient update in (7). Specifically, they are exactly equal if \( h_m(Y, X) = 1 \). Since in practice the update is usually damped, see Equation (16) in Section 2.4, and the shrinkage parameter \( \nu \) is considered a tuning parameter, the two approaches are essentially also equivalent for \( h_m(Y, X) = c \neq 1 \).

2.1.3 Hybrid gradient-Newton boosting

A hybrid variant of gradient and Newton boosting is obtained by first learning part of the parameters of the base learner using a gradient step and the remaining part using a Newton update. For instance, for trees as bases learners, the structure \( s \) of a tree is learned using a gradient update:

\[
    s_m = \arg\min_{s: f = w_s \in \mathcal{S}} E_{Y, X} \left( (-g_m(Y, X) - f(X))^2 \right),
\]

and then, conditional on this, one finds the weights \( w \) using a Newton step:

\[
    w_m = \arg\min_{w: f = w_s \in \mathcal{S}, s = s_m} E_{Y, X} \left( g_m(Y, X)f(X) + \frac{1}{2} h_m(Y, X)f(X)^2 \right).
\]

This is the approach proposed in [Friedman 2001].

2.1.4 Line search

The update step in (3) is sometimes presented in the form \( F_m(x) = F_{m-1}(x) + \rho_m f_m(x) \) with \( \rho_m \in \mathbb{R} \), where \( \rho_m \) is found by doing an additional line-search \( \rho_m = \arg\min_{\rho \in \mathbb{R}} R^e (F_{m-1} + \rho f_m) \).

We are not considering this approach explicitly here since, first, we assume that the set of base learners \( \mathcal{S} \) is rich enough to include not just normalized base learners but base learners of any norm and, second, the line-search often cannot be done analytically and a second-order Taylor approximation is used instead, which then corresponds to a Newton step. This means that the latter case is essentially a version of hybrid gradient-Newton or Newton boosting.

2.1.5 Applicability of Newton boosting

As mentioned in Section 2.1.2 there is no difference between the three above presented optimization approaches for loss functions with non-zero, constant second derivatives in \( F \). In particular, this holds true for the squared loss function.
Further, for loss functions where the second derivative is zero on a non-null set of the support of $X$, such as the least absolute deviation (LAD), any other quantile regression loss function, and the Huber loss, Newton and also hybrid gradient-Newton boosting is not applicable. In these cases, the above-mentioned line-search might be useful in addition to a pure gradient step. Similarly, if a loss function is not $P$-almost everywhere twice differentiable in $F$, Newton boosting is also not applicable. However, the majority of commonly used loss functions are twice differentiable.

2.2 Sample versions

In the following, we assume that we observe $n$ samples $(y_i, x_i), i = 1, \ldots, n$, from the same distribution as the one of $(Y, X)$, and approximate the risk $R(F)$ in (1) with the empirical risk $R^e(F)$:

$$R^e(F) = \sum_{i=1}^{n} L(y_i, F(x_i)).$$  \hspace{1cm} (11)

For gradient boosting, the sample version of (7) can be written as

$$f_m = \arg\min_{f \in S} \sum_{i=1}^{n} g_{m,i} f(x_i) + \frac{1}{2} f(x_i)^2$$

$$= \arg\min_{f \in S} \sum_{i=1}^{n} (-g_{m,i} - f(x_i))^2,$$  \hspace{1cm} (12)

where $g_{m,i}$ is the gradient of the loss function for observation $i$

$$g_{m,i} = \frac{\partial}{\partial F} L(y_i, F) \bigg|_{F=F_{m-1}(x_i)}.$$  \hspace{1cm} (13)

This means that the stagewise minimizer $f_m$ can be found as the least squares approximation to the negative gradient $-g_{m,i}$.

Similarly, the sample version of the Newton update in (9) is given by

$$f_m = \arg\min_{f \in S} \sum_{i=1}^{n} g_{m,i} f(x_i) + h_{m,i} \frac{1}{2} f(x_i)^2$$

$$= \arg\min_{f \in S} \sum_{i=1}^{n} h_{m,i} \left( -\frac{g_{m,i}}{h_{m,i}} - f(x_i) \right)^2,$$  \hspace{1cm} (14)

where $h_{m,i}$ is the Hessian of the loss function for observation $i$:

$$h_{m,i} = \frac{\partial^2}{\partial F^2} L(y_i, F) \bigg|_{F=F_{m-1}(x_i)}.$$  \hspace{1cm} (14)
I.e., $f_m$ can be found as the weighted least squares approximation to the ratio of the negative gradient over the Hessian $-\frac{g_{m,i}}{h_{m,i}}$ with weights given by $h_{m,i}$.

The sample version of the hybrid gradient-Newton algorithm first finds the structure $s$ of a tree using a gradient step:

$$s_m = \arg\min_{s:f=w_s\in S} \sum_{i=1}^n (-g_{m,i} - f(x_i))^2,$$

and then determines the weights $w$ using a Newton step:

$$w_m = \arg\min_{w:f=w_s\in S, s=s_m} \sum_{i=1}^n h_{m,i} \left( -\frac{g_{m,i}}{h_{m,i}} - f(x_i) \right)^2.$$

### 2.3 Multivariate case

In this section, we briefly present gradient and Newton boosting for the case where the function $F$ is multivariate. In this case,

$$F(X) = (F^1(X), F^2(X), \ldots, F^d(X))^T$$

is assumed to be a function in a direct sum Hilbert space $\mathcal{H} = \mathcal{H}^1 \oplus \mathcal{H}^2 \oplus \cdots \oplus \mathcal{H}^d$, where the $\mathcal{H}^k$'s are Hilbert spaces with inner products $\langle \cdot, \cdot \rangle_k$ given by $\langle F^k, F^k \rangle_k = E_X (F^k(X)^2)$, and the inner product for $\mathcal{H}$ is given by $\langle F, F \rangle = \sum_{k=1}^d \langle F^k, F^k \rangle_k$. For the sake of readability, we use boldface in this subsection to distinguish vector-valued functions from scalar-valued functions. Examples of loss functions where $F$ is multivariate include the entropy loss with a softmax function for multiclass classification or generalized additive models for location, scale and shape (GAMLSS) where location, scale, and shape parameters are modeled as functions of predictor variables $X$ [Rigby and Stasinopoulos, 2005; Mayr et al., 2012].

A gradient boosting update $f_m \in S \oplus \cdots \oplus S$ in Equation (3) is then obtained as

$$f_m = \arg\min_{f \in S \oplus \cdots \oplus S} dR(F_{m-1}, f) + \frac{1}{2} \langle f, f \rangle. \tag{15}$$

Under appropriate regularity conditions, $dR(F_{m-1}, f)$ is given by

$$dR(F_{m-1}, f) = E_{Y,X} \left( g_m(Y, X)^T f(X) \right),$$

where

$$g_m(Y, X) = \left( \frac{\partial}{\partial F^1} L(Y, F), \ldots, \frac{\partial}{\partial F^d} L(Y, F) \right)^T \bigg|_{F=F_{m-1}(X)}.$$
It follows that the solution in (15) can be determined for each \( k, k = 1, \ldots, d \), separately as

\[
  f^k_m = \arg\min_{f^k \in S} E_{Y,X} \left( \left( -g^k_m(Y,X) - f^k(X) \right)^2 \right),
\]

where

\[
  g^k_m(Y,X) = \frac{\partial}{\partial F^k} L(Y,F) \bigg|_{F = F_{m-1}(X)}.
\]

The sample version of this gradient boosting update is given by

\[
  f^k_m = \arg\min_{f^k \in S} \sum_{i=1}^n \left( -g^k_{m,i} - f^k(x_i) \right)^2,
\]

where \( g^k_{m,i} = g^k_m(y_i, x_i) \).

Newton boosting obtains an update \( f_m \in S \oplus \cdots \oplus S \) as

\[
  f_m = \arg\min_{f \in S \oplus \cdots \oplus S} dR(F_{m-1}, f) + \frac{1}{2} d^2 R(F_{m-1}, f),
\]

where, again under appropriate conditions, this can also be written as

\[
  f_m = \arg\min_{f \in S \oplus \cdots \oplus S} E_{Y,X} \left( g_m(Y,X)^T f(X) + \frac{1}{2} f(X)^T h_m(Y,X) f(X) \right)
\]

with \( h_m(Y,X) = [h_m(Y,X)]_{k,l}, k, l = 1, \ldots, d, \) and

\[
  [h_m(Y,X)]_{k,l} = \frac{\partial^2}{\partial F^k \partial F^l} L(Y,F) \bigg|_{F = F_{m-1}(X)}.
\]

The sample version of the Newton update is given by

\[
  f_m = \arg\min_{f \in S \oplus \cdots \oplus S} \sum_{i=1}^n g^T_{m,i} f(x_i) + \frac{1}{2} f(x_i)^T h_{m,i} f(x_i),
\]

where \( g_{m,i} = g_m(y_i, x_i) \) and \( h_{m,i} = h_m(y_i, x_i) \). In practice, one usually approximates \( h_{m,i} \) by a diagonal matrix

\[
  h_{m,i} \approx \text{diag} \left( \frac{\partial^2}{\partial F^k \partial F^l} L(Y,F) \right),
\]

i.e., one assumes that \( \frac{\partial^2}{\partial F^k \partial F^l} L(Y,F) = 0 \) for \( k \neq l \). In this case, the updates can be determined independently as

\[
  f^k_m = \arg\min_{f^k \in S} \sum_{i=1}^n h^k_{m,i} \left( -\frac{g^k_{m,i}}{h^k_{m,i}} - f^k(x_i) \right)^2,
\]

where \( h^k_{m,i} = h^k_m(y_i, x_i) \).
2.4 Tuning parameters and regularization

It has been empirically observed that damping the update in (3) results in increased predictive accuracy [Friedman, 2001]. This means that the update in (3) is replaced with

\[ F_m(x) = F_{m-1}(x) + \nu f_m(x), \quad \nu \in (0, 1], \]  

where the shrinkage parameter \( \nu \) is often denoted as learning rate. The parameter \( \nu \) can be thought of as a regularization parameter. Under additional assumptions, one can show [Efron et al., 2004, Zhao and Yu, 2007] that when the parameter \( \nu \) goes to zero, the obtained solutions correspond to the set of Lasso [Tibshirani, 1996] solutions.

The main tuning parameters of boosting algorithms are then the number of boosting iterations \( M \) and the shrinkage parameter \( \nu \). These tuning parameters and also the ones for the base learners presented in the following can be chosen by minimizing a performance measure on a validation dataset, by cross-validation, or using an appropriate model selection criterion.

2.4.1 The minimal equivalent number of weighted samples per leaf

Depending on the choice of base learners, there are additional tuning parameters. For instance, if trees are used as base learners, the depth of the trees \( L \) and the minimal number of samples per leaf are further tuning parameters. Since Newton boosting solves the weighted least squares problem in (13) in each update step, the raw number of samples per leaf is not meaningful, and we argue that instead, one should consider what we denote as the equivalent number of weighted samples per leaf. As we show below on real-world and simulated data, this parameter is important for predictive accuracy.

For gradient boosting or hybrid gradient-Newton boosting, every data point has a weight of one when learning the structure of a tree. Motivated by this, we first normalize the weights

\[ \tilde{w}_{m,i} = \frac{n \cdot h_{m,i}}{\sum_{j=1}^{n} h_{m,j}}, \]

such that the sum of all normalized weights \( \tilde{w}_{m,i} \) equals the number of data points \( n \). We then interpret the sum of all normalized weights \( \sum_{i \in L_j} \tilde{w}_{m,i} \) per leaf \( L_j \) as the equivalent number of weighted data points, and require that this is larger than a certain constant \( S \):

\[ \sum_{i \in L_j} \tilde{w}_{m,i} \geq S. \]  

(17)
The constant $S$ is considered as a tuning parameter analogous to the minimum number of samples per leaf in gradient boosting.

To the best of our knowledge, the only other software that implements Newton boosting is XGBoost [Chen and Guestrin 2016]. XGBoost handles this tuning parameter differently by requiring that the sum of all raw weights $h_{m,i}$ per leaf is larger than a certain constant which is by default one. According to the authors of XGBoost, the motivation for this is that for linear regression, “this simply corresponds to minimum number of instances needed to be in each node.” We argue that this is not an optimal choice for the following two reasons.

First, the second derivative $h_{m,i}$ of the loss function of a linear regression model with Gaussian noise

$$L(Y, F) = \frac{(Y - F)^2}{2\sigma^2}$$

equals one only if the noise variance $\sigma^2$ is one, $\sigma^2 = 1$, i.e., if one assumes a squared loss. Otherwise, the Hessian $h_{m,i}$ equals $\sigma^{-2}$. This means that the analogy to the linear regression case does not hold true in general. In contrast, our proposed normalized weights $\tilde{w}_{m,i}$ do indeed equal one for the linear regression case no matter what the noise variance is, and thus the sum of normalized weights $\sum_{i \in L_j} \tilde{w}_{m,i}$ equals the number of samples per leaf for the linear regression model also when $\sigma^2 \neq 1$. Second, as we show in our empirical study on both real-world and simulated datasets, the minimal sum of raw weights $\sum_{i \in L_j} h_{m,i}$ is a parameter that is difficult to tune in practice, and we obtain inferior predictive accuracy for the large majority of datasets. Related to this, the sum of normalized weights $\tilde{w}_{m,i}$ can be interpreted as the equivalent number of weighted samples per leaf, and one has good intuition concerning reasonable choices for this, which do not depend on the size of the data $n$. For the sum of raw weights, this is not the case.

In addition to the above-presented tuning parameters, one can consider further tuning parameters such as $L^1$ and/or $L^2$ regularization penalties on the tree weights, or an $L^0$ penalty on the number of leaves. Finally, boosting algorithms can also be made stochastic [Friedman 2002] by (sub-)sampling data points in each boosting iteration and variables in the tree algorithm as it is done for random forests. Due to the high computational cost

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2This constant is denoted by $\text{min\_child\_weight}$ in XGBoost (as of February 7, 2019).

3Unfortunately, this is not documented in the corresponding companion article [Chen and Guestrin 2016]. We gather this information from the online documentation https://xgboost.readthedocs.io/en/latest/parameter.html (retrieved on February 7, 2019).
when choosing tuning parameters using cross-validation and for better comparability, we are not considering these additional regularization options in this article.

### 2.5 Numerical stability and computational cost

As observed by Friedman et al. [2000] for the LogitBoost algorithm, i.e. Newton boosting for a Bernoulli likelihood with a logistic link function, numerical stability can be an issue for Newton boosting. Friedman et al. [2000] thus enforce a lower threshold on the second derivatives $h_{m,i}$ such that they are always strictly positive. Similarly, we also enforce a lower bound on $h_{m,i}$ at $10^{-20}$ in our implementation of Newton boosting.4

Concerning computational cost, the main cost of a boosting algorithm with trees as base learners results from growing the regression trees [Ke et al., 2017]. Consequently, the differences in computational times are marginal for the three versions of boosting presented in this article. Tree boosting implementations that are designed to scale to large data use computational tricks when growing trees; see, e.g., Chen and Guestrin [2016].

### 2.6 Software implementations

The methodology presented in this article, i.e., gradient, Newton, and hybrid gradient-Newton boosting is implemented in the Python package KTBoost, which is openly available from the Python Package Index (PyPI) repository.5

In the following, we briefly summarize which types of boosting algorithms are used by existing software implementations. The R package gbm [Ridgeway, 2007, 2017] and the Python library scikit-learn [Pedregosa et al., 2011] follow the approach of Friedman [2001] and use gradient descent steps for finding the structures of trees with Newton updates for the tree leaves (if applicable, see Section 2.1.5). Despite the name “eXtreme Gradient Boosting”, XGBoost [Chen and Guestrin, 2016] uses Newton boosting with Newton steps for finding both the tree structure and the tree leaves. The R package mboost [Hothorn et al., 2010] uses gradient boosting. In addition to trees, it also supports other base learners which

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4 We have not done a comprehensive study on the impact of this lower bound. However, when we choose the bounds at $10^{-16}$ and $10^{-30}$, we have not observed any noticeable differences in the outcomes (results not reported).

5 The parameter update_step of the functions BoostingClassifier and BoostingRegressor takes as arguments gradient, hybrid, or newton. E.g., for Newton boosting, one needs to choose the option update_step='newton'. See https://github.com/fabsig/KTBoost for more information.
include linear functions, one- and two-dimensional smoothing splines, spatial terms, as well as user-defined ones. Other recent implementations such as LightGBM [Ke et al., 2017], TF Boosted Trees [Ponomareva et al., 2017] and Spark MLLib [Meng et al., 2016], do not explicitly mention in their companion articles [Ke et al., 2017; Ponomareva et al., 2017] or in their online documentation[6] whether gradient descent or Newton updates are used in the stagewise boosting updates. Since Friedman [2001] is referenced in Ke et al. [2017] and Ponomareva et al. [2017], we assume that they use the hybrid gradient boosting approach of Friedman [2001] with Newton updates for the leaves. Finally, CatBoost [Prokhorenkova et al., 2018] uses gradient descent. To the best of our knowledge, none of the existing solutions allows the user to explicitly choose between a gradient or a Newton step for calculating the boosting updates.

3 Empirical evaluation and comparison

In the following, we compare the three different boosting algorithms presented in the previous section for different loss functions on various datasets. In doing so, we use regression trees as base learners. Specifically, we use the CART version of Breiman et al. [1984] with the mean squared error as splitting criterion. Note that we use trees [Breiman et al., 1984] as base learners as these are the most widely adopted base learners in applied data analysis and machine learning research [Ridgeway, 2017; Pedregosa et al., 2011; Chen and Guestrin, 2016; Meng et al., 2016; Ke et al., 2017; Ponomareva et al., 2017]. In addition, to Newton boosting with our novel equivalent number of weighted samples per leaf parameter as described in Section 2.4.1, we also consider Newton boosting as implemented in XGBoost for which the sum of Hessians in each leaf acts as tuning parameter (so called min_child_weight parameter)[7].

We consider the following datasets: adult, bank, (breast) cancer, ijcnn, ionosphere, titanic, sonar, car, covtype, digits, glass, letter, satimage, smartphone, usps, insurance, birthweight, and (childhood) malnutrition. Poisson regression is used for the insurance

[6]https://spark.apache.org/docs/latest/ml-classification-regression.html#gradient-boosted-trees-gbts (retrieved on February 7, 2019).

[7]We use XGBoost version number 0.7 in Python with the options tree_method='exact', updater='grow_colmaker', lambda=0, and all other parameters at the default values unless otherwise mentioned.
dataset. For the birthweight and malnutrition datasets, we use mean-scale regression assuming a normal likelihood where both the mean and the log-transformed scale parameter, i.e. the log-transformed standard deviation, are modeled as functions of the predictor variables; see Appendix A for more details. Note that the mean-scale regression model is an example of a GAMLSS model [Rigby and Stasinopoulos, 2005 Mayr et al., 2012]. For all remaining datasets, binary or multiclass classification is used. The insurance dataset is obtained from Kaggle.8 The birthweight [Schild et al., 2008] and malnutrition [Fenske et al., 2011] datasets are obtained from the tbm R package.9 The covtype, icnn, and usps datasets are LIBSVM datasets.10 All other datasets are obtained from the UCI Machine Learning Repository.11 A summary of the datasets can be found in Table 1. If a dataset contains categorical predictor variables, these are converted to binary dummy variables using one-hot encoding.

We randomly split the data into three equally sized datasets: training, validation, and test data. Learning is done on the training data, tuning parameters are chosen on the validation data, and model comparison is done on the test data. For the two largest datasets (icnn and covtype) we limit the size of the training, validation, and test data to 20000 data points. This is done for computational reasons. We note that there are various strategies in order that tree-based boosting scales to large data [Chen and Guestrin, 2016, Ke et al., 2017], but this is out of the scope of this article. In order to quantify variability in the results, we use several different random splits of the data. The number of sample splits is 100 for datasets with less than 1500 samples (less than 500 training samples), 20 for datasets with a size between 1500 and 7500 (number of training samples between 500 and 2500), and 10 for datasets with more than 7500 samples (more than 2500 training samples).

Concerning tuning parameters, we select the number of boosting iterations \( M \) from \{1, 2, \ldots, 1000\}, the learning rate \( \nu \) from \{1, 10^{-1}, 10^{-2}, 10^{-3}\}, and the minimum number of samples per leaf from \{1, 5, 25, 100\}. For Newton boosting, the latter is replaced by the equivalent number of weighted samples in Equation (17), and for the XGBoost implementation, the minimum sum of Hessians per leaf is used. Further, for the mean-scale regression datasets, the minimum number of samples per leaf is chosen from \{25, 100\} only for gra-

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8https://www.kaggle.com/apex51/poisson-regression
9Available on https://r-forge.r-project.org
10Obtained from https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/
11http://archive.ics.uci.edu/ml/datasets/
Gradient and hybrid boosting since a very small number of samples can lead to identifiability problems when modeling both the mean and the scale. Tuning parameters are chosen for each sample split such that they minimize the error rate for classification and the negative log-likelihood for regression on the validation data. The maximal tree depth is set to five for all methods. We are not considering the maximal tree depth as an additional tuning parameter for computational reasons\cite{12} and since fixing the maximal tree depth allows for a fairer comparison as all methods then use the same degree of interaction. However, additional results for a subset of the datasets reported in Section 5.1.2 and Appendix C show that similar findings are obtained for other tree depths. Note that in Section 5.1.1 and Appendix B we also consider the case when the minimum number of samples per leaf

\footnote{Having one tuning parameter less decreases the computational time required for evaluating a large number of datasets.}

| Data      | Type / nb. classes | Nb. samples | Nb. features |
|-----------|--------------------|-------------|--------------|
| adult     | 2                  | 48842       | 108          |
| bank      | 2                  | 41188       | 62           |
| cancer    | 2                  | 699         | 9            |
| ijcnn     | 2                  | 141691      | 22           |
| ionosphere| 2                  | 351         | 34           |
| sonar     | 2                  | 208         | 60           |
| car       | 4                  | 1728        | 21           |
| covtype   | 7                  | 581012      | 54           |
| digits    | 10                 | 5620        | 64           |
| glass     | 7                  | 214         | 9            |
| letter    | 26                 | 20000       | 16           |
| satimage  | 6                  | 6438        | 36           |
| smartphone| 6                  | 10299       | 561          |
| usps      | 10                 | 9298        | 256          |
| insurance | Poisson regr.      | 50999       | 117          |
| birthweight| Mean-scale regr. | 150         | 5            |
| malnutrition | Mean-scale regr. | 24166       | 42          |

Table 1: Summary of datasets.
parameter is not chosen by cross-validation and set to a default value, and we find very similar results.

| Data  | CompareAll | NewtonVsGrad | NewtonVsHybrid | NewtonVsXGBoost |
|-------|------------|--------------|----------------|-----------------|
| adult | 0.316      | 0.116        | 0.321          | 0.0488          |
| bank  | 0.143      | 0.404        | 0.215          | 0.0189          |
| cancer| 0.292      | 0.0681       | 0.304          | 0.47            |
| ijcnn | 1.91e-11   | 2.25e-06     | 0.000201       | 0.000346        |
| ionosphere | 0.00142   | 0.00711      | 0.15           | 0.000604        |
| sonar | 0.0228     | 0.0159       | 0.0379         | 0.00914         |
| car   | 1.21e-05   | 0.0209       | 0.402          | 0.000329        |
| covtype | 8.32e-09  | 4.57e-06     | 0.00028        | 1.26e-06        |
| digits| 0          | 8.21e-10     | 0.000189       | 3.01e-11        |
| glass | 0.0396     | 0.814        | 0.21           | 0.0991          |
| letter | 4.44e-16   | 1.64e-08     | 6.3e-06        | 6.27e-06        |
| satimage | 1.43e-09  | 2.55e-07     | 0.000581       | 0.00026         |
| smartphone | 6.42e-10 | 3.93e-05     | 1.7e-05        | 9e-06           |
| usps  | 2e-14      | 2.28e-06     | 3.27e-06       | 2.18e-07        |
| insurance | 0      | 0.0727       | 0.091          | 2.57e-09        |
| malnutrition | 0     | 3.55e-15     | 0.254          |                 |
| birthweight | 0     | 0            | 0.145          |                 |

Table 2: Comparison of different boosting methods using test error rates for classification and test negative log-likelihoods for regression. The column 'CompareAll' contains p-values of F-tests that compare differences among all methods. The other columns contain p-values of t-tests comparing Newton boosting with our novel tuning parameter to the other boosting variants. Random effects are used to account for correlation among the results for different sample splits.

In Figure [1] and Table [2], we report the results. We use the test error rate for classification and the out-of-sample negative log-likelihood on the test data for regression datasets to compare the different methods. Figure [1] visualizes the results using boxplots. The red rhombi represent means over the different sample splits. To investigate whether the differences are significant, we additionally report in Table [2] p-values when comparing the
Figure 1: Comparison of boosting methods using out-of-sample error rate for classification and negative log-likelihood for regression. The red rhombi represent means.
four methods. The column ‘CompareAll’ contains p-values of F-tests that compare differences among all four approaches. The other columns contain p-values of t-tests comparing Newton boosting to the other boosting variants as well as the XGBoost implementation of Newton boosting which uses the minimum number of Hessians per leaf as a tuning parameter. All tests are done using a regression model with a random effect at the sample split level to account for correlation among the results for different sample splits.

We observe substantial differences in the performance of the different methods. In general, we find that Newton boosting performs best, followed by hybrid gradient-Newton boosting. Gradient boosting often has the lowest predictive accuracy. Specifically, Figure 1 shows that Newton boosting has the highest predictive accuracy for the large majority of classification datasets with particularly striking differences for the following datasets: ijcnn, digits, letter, satimage, smartphone, and usps. For the two regression datasets where mean-scale regression is used (birthweight and malnutrition), we also observe that gradient boosting performs worse than Newton and hybrid gradient-Newton boosting, but no notable difference among the latter two is found. For the Poisson regression dataset (insurance), gradient, hybrid, and Newton boosting perform equally well. In addition, Newton boosting with the equivalent number of weighted samples parameter performs substantially better than the XGBoost variant of Newton boosting with a minimal sum of Hessians parameter.

Concerning statistical significance, there are significant differences at the 5% level in the accuracy of the different boosting variants for fifteen out of seventeen datasets. Further, Newton boosting is significantly better than gradient boosting for eleven datasets and also better than the hybrid version for eight datasets. In particular, there is no dataset for which either gradient boosting or the hybrid boosting version has significantly higher predictive accuracy than Newton boosting. In addition, Newton boosting with the novel equivalent number of weighted samples parameter performs significantly better than the XGBoost variant of Newton boosting with a minimal sum of Hessians parameter for the large majority of the datasets (twelve).

\[13\text{It is not entirely clear whether this difference is only due to the fact that XGBoost has a different minimum number of weighted samples parameter. Other implementation details, which are not clearly documented in the companion article of XGBoost [Chen and Guestrin, 2016], such as, e.g., split finding and ways to handle numerical overflows might also contribute.}\]
4 Simulation study

In the following, we also compare the performance of the different boosting approaches on simulated data for both classification and regression. Concerning regression, we consider two extensions of generalized linear models [McCullagh and Nelder 1989], boosted Poisson and Gamma regression, as well as the mean-scale regression model used in Section 3. For classification, we consider both binary and multiclass classification. In addition, we consider the boosted Tobit model [Sigrist and Hirnschall 2017], which can be considered as a hybrid regression-classification model. See Section A in the appendix for more details on these models.

For Poisson and Gamma regression, the boosted Tobit model, as well as mean-scale regression (‘msr’), we use the functions ‘make_friedman1’ and ‘make_friedman3’ available in scikit-learn and introduced in Friedman [1991] and Breiman [1996]. They are given by

\[ F(X) = 10 \sin(\pi X_1 X_2) + 20(X_3 - 0.5)^2 + 10X_4 + 5X_5 \quad (‘f1’), \]

where \( X = (X_1, \ldots, X_{10})' \), \( X_j \sim Unif(0,1) \), independent, and

\[ F(X) = 5 \cdot \tan^{-1} \left( \frac{X_2 X_3 - 1}{X_1 X_4} \right) + 0.2 \quad (‘f3’), \]

where \( X = (X_1, X_2, X_3, X_4)' \) with

\[ X_1 \sim Unif(0,100), \quad X_2 \sim Unif(40\pi,560\pi), \quad X_3 \sim Unif(0,1), \quad X_4 \sim Unif(1,11). \]

In contrast to the original function of Friedman [1991], we multiply the friedman3 function by 5 and add 0.2. The former is done in order that the function also contains larger values and the latter in order that all values are positive. We denote datasets generated by these two functions using the suffixes ‘_f1’ and ‘_f3’ in the following. In addition, we also consider the following function introduced in Ridgeway [1999]:

\[ F(X) = \exp \left( 2 \sin(3X_1 + 5X_1^2) - 2 \sin(3(X_2 + 0.1) + 5(X_2 + 0.1)^2) \right) \quad (‘r’), \]

where \( X = (X_1, X_2)' \), \( X_j \sim Unif(0,1) \), independent. Datasets generated using this function are denoted by the suffix ‘_r’.[14] For Poisson and Gamma regressions, the above functions are used to model then mean, and for Tobit regression the functions model the mean of

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[14]For instance, the dataset ‘msr_r’ is simulated from a mean-scale regression model with both the mean and the standard deviation given by the above function introduced by [Ridgeway 1999].
the latent variable. For the mean-scale regression model, we simulate $2p$ variables and relate both the mean and the logarithmic standard deviation to half of the $2p$ variables using the above functions. Both Tobit regression and a regression model where both the mean and the scale depend on predictor variables are not supported in XGBoost and, consequently, no comparison can be done for these cases.

For Gamma regression, we set the shape parameter to $\gamma = 10$ and consider this as a known parameter. For the Tobit model, we use $\sigma = 1$ and also consider this as a known parameter. Further, we set the lower and upper censoring thresholds $y_l$ and $y_u$ in such a way that approximately one-third of all data points are lower and upper censored.

For classification, we use the scikit-learn function `make_classification`, which simulates from an algorithm that is adapted from [Guyon 2003] and was designed to generate the ‘Madelon’ dataset. We use this for both simulating binary data and a multiclass data with five classes. Further, we assume ten (informative) features and no redundant and repeated features; see [Guyon 2003] for more details. These two datasets are denoted by ‘bin_classif’ and ‘multi_classif’ in the following. In addition, we simulate binary data according to the following specification introduced in [Friedman et al., 2000]:

$$Y|X \sim \text{Bernoulli}(p), \quad p = \left(1 + e^{-F(X)}\right)^{-1},$$

$$F(X) = 10 \sum_{j=1}^{6} X_j \left(1 + \sum_{l=1}^{6} (-1)^l X_l \right),$$

$$X \sim N(0, I_{10}).$$

This data is denoted by ‘bin_classif_fht’ in the following. Finally, we also simulate multiclass data with five classes according to the following specification [Friedman et al., 2000]:

$$R^2 = \sum_{j=1}^{10} X_j^2,$$

$$Y = k \quad \text{if} \quad t_k \leq R^2 < t_{k+1},$$

$$X \sim N(0, I_{10}),$$

where the thresholds $t_k$ are chosen such that the labels are approximately equally distributed among the different classes. We denote this data by ‘multi_classif_fht’.

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15 We note that XGBoost only supports Gamma regression for $\gamma = 1$. However, this slight misspecification seems to have no detrimental impact as our results below show.
We simulate 10 times datasets with 15000 samples. In each run, 5000 samples are used as training, validation, and test data. The results from this are reported in Figure 2. In Table 3, we report p-values of tests in order to check whether there are significant differences among the different boosting approaches and whether Newton boosting performs better than the other versions. See Section 3 for more details on the plots and tests.

| Data          | CompareAll | NewtonVsGrad | NewtonVsHybird | NewtonVsXGBoost |
|---------------|------------|--------------|----------------|----------------|
| bin_classif   | 2.72e-07   | 3.11e-05     | 5.2e-05        | 0.00532        |
| bin_classif_fht | 0.175      | 0.374        | 0.327          | 0.395          |
| multi_classif | 1.54e-10   | 1.08e-05     | 2.57e-05       | 0.207          |
| multi_classif_fht | 0         | 9.58e-12     | 6.02e-11       | 2.83e-09       |
| poisson_r     | 1.22e-07   | 4.89e-05     | 0.00137        | 0.132          |
| poisson_f1    | 5.63e-09   | 6.17e-06     | 0.0269         | 0.0214         |
| poisson_f3    | 6.07e-10   | 3.29e-05     | 0.000579       | 0.463          |
| gamma_r       | 0.0793     | 0.0504       | 0.0208         | 0.0705         |
| gamma_f1      | 0.0875     | 0.0319       | 0.193          | 0.213          |
| gamma_f3      | 1.15e-05   | 0.000153     | 0.161          | 0.0274         |
| tobit_r       | 4.97e-05   | 0.000445     | 0.118          |                |
| tobit_f1      | 0.356      | 0.228        | 0.794          |                |
| tobit_f3      | 4.51e-06   | 5.33e-06     | 0.0123         |                |
| msr_f1        | 0          | 5.47e-12     | 0.368          |                |
| msr_f3        | 2.64e-13   | 5.86e-08     | 0.00583        |                |
| msr_r         | 1.76e-13   | 4.18e-08     | 0.0163         |                |

Table 3: Comparison of different boosting methods using test error rates for classification and test negative log-likelihoods for regression.

For the majority of the datasets, we find statistically significant differences among the different boosting approaches. As in Section 3, we find again that Newton boosting usually performs best, followed by hybrid gradient-Newton, with gradient boosting having the lowest predictive accuracy. In particular, Newton boosting performs significantly better at the 5% level than gradient boosting for all except three datasets and significantly better than hybrid gradient-Newton boosting for eight datasets. Finally, Newton boosting with the new equivalent sample size per leaf tuning parameter performs better than the XGBoost
Figure 2: Comparison of boosting methods on simulated datasets using out-of-sample error rate for classification and negative log-likelihood for regression. The red rhombi represent means.

implementation for most datasets.
5 Why does Newton boosting outperform gradient boosting?

In the previous sections, we empirically show that Newton boosting results in better predictive accuracy than gradient and hybrid gradient-Newton boosting for many datasets including classification and regression tasks with both multivariate as well as one-dimensional parameters modeled as ensembles of trees. In the following, we shed some light on why we observe these differences.

A straightforward explanation for the observed phenomenon is that Newton boosting learns faster than both gradient and hybrid gradient-Newton boosting, and that hybrid boosting also learns faster than gradient boosting. To investigate whether this is the main reason for the differences, we show in Figures 3 and 4 test error rates (classification) and test negative log-likelihoods (regression) as well as training losses versus iteration numbers for several datasets for which we observe the large differences. In order that the results for the different sample splits and also boosting methods are comparable, learning rates are fixed and not tuned. Specifically, we consider the following datasets and learning rates: ijcnn ($\nu = 0.5$), bin_classif ($\nu = 0.5$), digits ($\nu = 0.5$), letter ($\nu = 0.1$), satimage ($\nu = 0.3$), smartphone ($\nu = 0.5$), poisson_r ($\nu = 0.03$), malnutrition ($\nu = 0.03$), and mshr_r ($\nu = 0.05$). Note that this list of datasets includes both binary and multiclass classification as well as Poisson and mean-scale regression tasks. The solid lines in Figures 3 and 4 represent means over ten different data splits into equally sized training, validation, and test data. The lower and upper values are obtained after point-wise discarding the lowest and largest values. Training losses are shown on a logarithmic scale with a lower cap at $10^{-5}$ for better visualization.

As expected, Figures 3 and 4 show that gradient boosting often converges slower than Newton and also hybrid gradient-Newton boosting. Concerning the latter two, we visually observe no difference in convergence speed. Interestingly, the figures clearly show that Newton boosting achieves both lower training losses as well as lower test errors than gradient and hybrid gradient-Newton boosting for all classification datasets. In fact, the training losses of Newton boosting converge to zero up to machine precision for all multiclass classification datasets (digits, letter, satimage, and smartphone) and to values below $1^{-15}$ for the two binary classification datasets (ijcnn and bin_classif). Further, hybrid gradient-Newton
boosting also results in both lower training losses and test errors than gradient boosting for the classification datasets\textsuperscript{16}. For the Poisson regression dataset, we observe similar results with the difference that gradient boosting results in a lower training loss but a higher test loss. For the mean-scale regression datasets, we observe that Newton and hybrid boosting show lower test and training losses than gradient boosting. In contrast to the classification

\textsuperscript{16}Note that for a few datasets (e.g., bin\_classif, letter), the test error rates of gradient boosting have not yet fully converged to their minima for the chosen learning rates. Nonetheless, we stop after 1000 iterations for computational reasons. For better comparability, we use the same learning rate for all methods.
datasets, we find clear signs of overfitting as the test losses start to increase again after a certain number of boosting iterations for the mean-scale regression datasets. Concerning the XGBoost implementation, we find that the XGBoost result in larger training losses and also larger test errors compared to our Newton boosting implementation. In particular, the training losses do not converge to zero for the classification datasets.

In summary, our experiments show that convergence speed is not the main reason for the observed differences in predictive accuracy. Interestingly, our results indicate that Newton
boosting converges to lower training losses, which are essentially zero for the majority of
classification datasets, while at the same time having higher out-of-sample accuracy. The
fact that interpolating classifiers with zero training loss generalize well to novel data seems
to be in contradiction to the well-known bias-variance trade-off. However, similar results
have recently been observed for other datasets and complex models such as deep learning
and kernel machines [Zhang et al., 2017, Belkin et al., 2018b,a].

Finally, we recall that in cases where the Hessians $h_{m,i}$ defined in Equation (14) are
constant, there is no difference between gradient and Newton boosting. It is thus likely
that the more variation there is in the second order terms $h_{m,i}$ the larger is the difference
between gradient and Newton boosting.

5.1 Additional results

In the following, we report additional results to show that our findings are robust to the
choice of tuning parameters.

5.1.1 No tuning for the minimum number of (weighted) samples parameter

In Appendix B in Figure 5 and Table 4 we also report the results for the real-world datasets
when the minimum number of (weighted) samples per leaf parameter is not chosen using
cross-validation and simply set to the default value. I.e., for gradient and hybrid gradient-
Newton boosting, the minimum number of samples per leaf is one, for Newton boosting with
our proposed choice in (17), we set the minimum equivalent number of weighted samples
per leaf to one, and for the XGBoost implementation, we set the minimum sum of Hessians
to its default value, i.e., also one.$^{17}$

Overall, we find that the difference in predictive accuracy between Newton boosting
and gradient as well as hybrid gradient-Newton boosting is even more pronounced when
the minimum number of samples parameter is not tuned.

5.1.2 Maximal tree depth

We also consider other maximal tree depths for a subset of the datasets. Specifically, we
additionally use the following maximal tree depths: 1 (stumps), 3, 8, and 20. The results in

$^{17}$ We exclude the mean-scale regression datasets as there is no obvious default value since the minimum
number of samples per leaf needs to be larger than one.
Appendix C show that we continue to observe very similar differences among the different boosting versions also for other maximal tree depths. For the majority of the datasets, stumps and also trees with maximal depth 3 perform worse than larger trees. For one simulated dataset (multi_classif_fht), stumps result in increased predictive accuracy. In general, we observe only minor differences if we set the maximal tree depth to either 5, 8, or 20.

6 Conclusions

We compare gradient and Newton boosting as well as a hybrid variant of the two with trees as base learners on a wide range of classification and regression datasets. Our empirical results show that Newton boosting outperforms gradient and often also hybrid gradient-Newton boosting. Further, we show evidence that this outperformance is not primarily due to faster convergence speed but due to the fact that tree-based Newton boosting converges to lower values of the empirical risk while at the same time having lower test errors. Future research should shed light on the reasons for this. Further, it remains to be investigated whether similar results are found for other types of base learners such as splines [Bühlmann and Yu 2003, Hothorn et al. 2010] or reproducing kernel Hilbert space (RKHS) regression functions [Sigrist 2019].

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Appendices

A Loss functions for regression and classification tasks

In the following, we list the loss functions and corresponding gradients and second derivatives that we consider in this article.

- **Binary classification**
  \[ Y|X \sim \text{Bernoulli}(p), \quad p = (1 + e^{-F(X)})^{-1} \]
  Loss: \( L(Y, F) = -YF + \log(1 + e^F) \)
  Gradient: \( \frac{\partial}{\partial F} L(Y, F) = -Y + p \)
  Hessian: \( \frac{\partial^2}{\partial F^2} L(Y, F) = p(1 - p) \)

- **Multiclass classification**
  \[ Y|X \sim \text{Multinom}(p_1, \ldots, p_K), \quad p_k = \frac{e^{F_k(X)}}{\sum_{l=1}^{K} e^{F_l(X)}}, \quad k = 1, \ldots, K \]
  Loss: \( L(Y, F) = \sum_{k=1}^{K} \left( -1_{\{Y=k\}} F_k + \log \left( \sum_{l=1}^{K} e^{F_l(X)} \right) \right), \quad F = (F_1, \ldots, F_K) \)
  Gradient: \( \frac{\partial}{\partial F_k} L(Y, F) = -1_{\{Y=k\}} + p_k \)
  Hessian: \( \frac{\partial^2}{\partial F_k^2} L(Y, F) = p_k(1 - p_k) \)
  As in Friedman et al. [2000], we use \( \frac{\partial^2}{\partial F_k \partial F_j} L(Y, F) = 0 \) for simplicity.

- **Poisson regression**
  \[ Y|X \sim \text{Pois}(\lambda), \quad \lambda = e^{F(X)} \]
  Loss: \( L(Y, F) = -YF + e^F \)
  Gradient: \( \frac{\partial}{\partial F} L(Y, F) = -Y + e^F \)
  Hessian: \( \frac{\partial^2}{\partial F^2} L(Y, F) = e^F \)

- **Gamma regression**
  \[ Y|X \sim \text{Gamma}(\gamma, \lambda) \text{ with shape } \gamma \text{ and rate } \lambda, \quad \lambda = \gamma e^{-F(X)} \]
  Loss: \( L(Y, F) = \gamma \left( F + e^{-F}Y \right) - (\gamma - 1) \log(Y) - \gamma \log(\gamma) + \log(\Gamma(\gamma)) \)
  Gradient: \( \frac{\partial}{\partial F} L(Y, F) = \gamma \left( 1 - e^{-F}Y \right) \)
  Hessian: \( \frac{\partial^2}{\partial F^2} L(Y, F) = \gamma e^{-F}Y \)

- **Tobit model**
  \[ Y|X \sim \text{Tobit}_{(y_l, y_u)}(\mu, \sigma^2), \text{ with mean } \mu, \ \mu = F(X), \text{ and variance } \sigma^2 \text{ of the latent variable and lower and upper censoring thresholds } y_l \text{ and } y_u \]
Loss: 
\[ L(Y, F) = -\log \left( \Phi \left( \frac{y_l - F}{\sigma} \right) \right) 1_{y_l}(Y) + \left( \frac{(Y - F)^2}{2\sigma^2} + \log(\sigma) + 0.5 \log(2\pi) \right) 1_{y_l < Y < y_u} \]
\[ - \log \left( 1 - \Phi \left( \frac{y_u - F}{\sigma} \right) \right) 1_{y_u}(Y) \]

Gradient: 
\[ \frac{\partial}{\partial F} L(Y, F) = \frac{\phi \left( \frac{y_l - F}{\sigma} \right)}{\sigma \Phi \left( \frac{y_l - F}{\sigma} \right)} 1_{y_l}(Y) - \frac{Y - F}{\sigma^2} \cdot 1_{y_l < Y < y_u} - \frac{\phi \left( \frac{y_u - F}{\sigma} \right)}{\sigma \left( 1 - \Phi \left( \frac{y_u - F}{\sigma} \right) \right)} 1_{y_u}(Y) \]

Hessian: 
\[ \frac{\partial^2}{\partial F^2} L(Y, F) = \frac{\phi \left( \frac{y_l - F}{\sigma} \right)}{\sigma^2 \Phi \left( \frac{y_l - F}{\sigma} \right)} \left( \frac{y_l - F}{\sigma} \Phi \left( \frac{y_l - F}{\sigma} \right) + \phi \left( \frac{y_l - F}{\sigma} \right) \right) 1_{y_l}(Y) + \frac{1}{\sigma^2} 1_{y_l < Y < y_u} \]
\[ - \frac{\phi \left( \frac{y_u - F}{\sigma} \right)}{\sigma^2 \left( 1 - \Phi \left( \frac{y_u - F}{\sigma} \right) \right)^2} \left( \frac{y_u - F}{\sigma} \left( 1 - \Phi \left( \frac{y_u - F}{\sigma} \right) \right) - \phi \left( \frac{y_u - F}{\sigma} \right) \right) 1_{y_u}(Y) \]

- Mean-scale regression

\( Y | X \sim N(\mu, \sigma^2) \), with mean \( \mu = F_1(X) \) and standard deviation \( \sigma = e^{F_2(X)} \)

Loss: 
\[ L(Y, F) = \frac{(Y - F_1)^2}{2e^{2F_2}} + F_2 + 0.5 \log(2\pi) \]

Gradient:
\[ \frac{\partial}{\partial F_1} L(Y, F) = -\frac{Y - F_1}{e^{2F_2}} \]
\[ \frac{\partial}{\partial F_2} L(Y, F) = -\frac{(Y - F_1)^2}{e^{2F_2}} + 1 \]

Hessian:
\[ \frac{\partial^2}{\partial F_1^2} L(Y, F) = \frac{1}{e^{2F_2}} \]
\[ \frac{\partial^2}{\partial F_2^2} L(Y, F) = \frac{2(Y - F_1)^2}{e^{2F_2}} \]

Similarly as for multiclass classification, we assume for simplicity zero off-diagonals for the Hessian, i.e., 
\( \frac{\partial^2}{\partial F_1 \partial F_2} L(Y, F) = 0 \).

B Results when the default value for the minimum number of (weighted) samples per leaf parameter is used
Figure 5: Comparison of boosting methods using out-of-sample error rate for classification and negative log-likelihood for regression. The minimum number of (weighted) samples parameter is set to the default value and not chosen using cross-validation.
| Data     | CompareAll | NewtonVsGrad | NewtonVsHybird | NewtonVsXGBoost |
|----------|------------|--------------|----------------|-----------------|
| adult    | 0.103      | 0.0234       | 0.885          | 0.842           |
| bank     | 0.017      | 0.143        | 0.765          | 0.0329          |
| cancer   | 0          | 4.84e-11     | 0.00013        | 7.62e-08        |
| ijcnn    | 3.22e-15   | 2.72e-07     | 1.05e-05       | 0.231           |
| ionosphere | 1.7e-12   | 1.68e-06     | 0.000628       | 0.0586          |
| sonar    | 0          | 0.000273     | 0.00021        | 4.3e-08         |
| car      | 4.46e-11   | 1.59e-07     | 3.67e-05       | 0.0721          |
| covtype  | 5.14e-11   | 1.57e-07     | 5.06e-06       | 1.77e-05        |
| digits   | 0          | 3.33e-16     | 7.22e-15       | 1.32e-06        |
| glass    | 1.47e-09   | 3.67e-06     | 0.0047         | 0.121           |
| letter   | 0          | 1.76e-09     | 8.27e-09       | 4.71e-05        |
| satimage | 0          | 7.73e-11     | 2.38e-07       | 0.000538        |
| smartphone | 0        | 2.13e-07     | 5.17e-06       | 0.000283        |
| usps     | 0          | 2.55e-10     | 6.74e-08       | 2.7e-06         |
| insurance | 0        | 3.4e-05      | 0.000222       | 2.52e-10        |

Table 4: Comparison of different boosting methods using test error rates for classification and test negative log-likelihoods for regression. The minimum number of (weighted) samples per leaf parameter is set to the default value and no tuning is done for this parameter.
C Results for different maximal tree depths

Figure 6: Results when the maximal tree depth is one (stumps).

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Figure 7: Results when the maximal tree depth is three.
Figure 8: Results when the maximal tree depth is eight.
Figure 9: Results when the maximal tree depth is 20.