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# Don't Sweat the Solver Stuff

Tips for Better Logistic Regression Models in Scikit-Learn



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Lighthouses Give Warnings

Logistic regression is the bread-and-butter algorithm for machine learning classification. If you're a practicing or aspiring data scientist, you'll want to know the ins and outs of how to use it. Also, Scikit-learn's `LogisticRegression` is spitting out

warnings about changing the default solver, so this is a great time to learn when to use which solver. 😊

```
FutureWarning: Default solver will be changed to 'lbfgs' in 0.22.  
Specify a solver to silence this warning.
```

In this article, you'll learn about Scikit-learn `LogisticRegression` solver choices and see two evaluations of them. Also, you'll see key API options and get answers to frequently asked questions. By the end of the article, you'll know more about logistic regression in Scikit-learn and not sweat the solver stuff. 😊

I'm using Scikit-learn version 0.21.3 in this analysis.

**UPDATE December 20, 2019:** I made several edits to this article after helpful feedback from Scikit-learn core developer and maintainer, Andreas Mueller.

## When to use Logistic Regression

A classification problem is one in which you try to predict discrete outcomes, such as whether someone has a disease. In contrast, a regression problem is one in which you are trying to predict a value of a continuous variable, such as the sale price of a home. Although logistic regression has *regression* in its name, it's an algorithm for classification problems.

Logistic regression is probably the most important supervised learning classification method. It's a fast, versatile extension of a generalized linear model.

Logistic regression makes an excellent baseline algorithm. It works well when the relationship between the features and the target aren't too complex.

Logistic regression produces feature weights that are generally interpretable, which makes it especially useful when you need to be able to explain the reasons for a decision. This interpretability often comes in handy — for example, with lenders who need to justify their loan decisions.

There is no closed-form solution for logistic regression problems. This is fine — we don't use the closed form solution for linear regression problems anyway because it's slow. 😊

Solving logistic regression is an optimization problem. Thankfully, nice folks have created several solver algorithms we can use. 😊

## Solver Options

Scikit-learn ships with five different solvers. Each solver tries to find the parameter weights that minimize a cost function. Here are the five options:

- `newton-cg` — A newton method. Newton methods use an exact Hessian matrix. It's slow for large datasets, because it computes the second derivatives.
- `lbfgs` — Stands for Limited-memory Broyden–Fletcher–Goldfarb–Shanno. It approximates the second derivative matrix updates with gradient evaluations. It stores only the last few updates, so it saves memory. It isn't super fast with large data sets. It will be the default solver as of Scikit-learn version 0.22.0.
- `liblinear` — Library for Large Linear Classification. Uses a coordinate descent algorithm. Coordinate descent is based on minimizing a multivariate function by solving univariate optimization problems in a loop. In other words, it moves toward the minimum in one direction at a time. It is the default solver for Scikit-learn versions earlier than 0.22.0. It performs pretty well with high dimensionality. It does have a number of drawbacks. It can get stuck, is unable to run in parallel, and can only solve multi-class logistic regression with one-vs.-rest.
- `sag` — Stochastic Average Gradient descent. A variation of gradient descent and incremental aggregated gradient approaches that uses a random sample of previous gradient values. Fast for big datasets.
- `saga` — Extension of `sag` that also allows for L1 regularization. Should generally train faster than `sag`.

An excellent discussion of the different options can be found in [this Stack Overflow answer](#).

The chart below from the [Scikit-learn documentation](#) lists characteristics of the solvers, including the the regularization penalties available.

Penalties	'liblinear'	'lbfgs'	'newton-cg'	'sag'	'saga'
Multinomial + L2 penalty	no	yes	yes	yes	yes
OVR + L2 penalty	yes	yes	yes	yes	yes
Multinomial + L1 penalty	no	no	no	no	yes
OVR + L1 penalty	yes	no	no	no	yes
Elastic-Net	no	no	no	no	yes
No penalty ('none')	no	yes	yes	yes	yes
Behaviors					
Penalize the intercept (bad)	yes	no	no	no	no
Faster for large datasets	no	no	no	yes	yes
Robust to unscaled datasets	yes	yes	yes	no	no

## Why is the default solver changing?

`liblinear` is fast with small datasets, but has problems with saddle points and can't be parallelized over multiple processor cores. It can only use one-vs.-rest to solve multi-class problems. It also penalizes the intercept, which isn't good for interpretation.

`lbfgs` avoids these drawbacks and is relatively fast. It's the best choice for most cases without a really large dataset. Some discussion of why the default was changed is in [this GitHub issue](#).

Let's evaluate the Logistic Regression solvers with two prediction classification projects — one binary and one multi-class.

## Solver Tests

### Binary classification solver example

First, let's look at a binary classification problem. I used the built-in [scikit-learn breast\\_cancer dataset](#). The goal is to predict whether a breast mass is cancerous.





The features consist of numeric data about cell nuclei. They were computed from digitized images of biopsies. The dataset contains 569 observations and 30 numeric features. I split the dataset into training and test sets and conducted a grid search on the training set with each different solver. You can access my Jupyter notebook used in all analyses on [Kaggle](#).

The most relevant code snippet is below.

```
solver_list = ['liblinear', 'newton-cg', 'lbfgs', 'sag', 'saga']
params = dict(solver=solver_list)
log_reg = LogisticRegression(C=1, n_jobs=-1, random_state=34)
clf = GridSearchCV(log_reg, params, cv=5)
clf.fit(X_train, y_train)
scores = clf.cv_results_['mean_test_score']

for score, solver in zip(scores, solver_list):
    print(f" {solver} {score:.3f}" )
```

And here are the results:

```
liblinear 0.939
newton-cg 0.939
```

```
lbfgs 0.934
sag 0.911
saga 0.904
```

The accuracy values for *sag* and *saga* are a bit lower than their peers.

After scaling the features, the solvers all perform better and *sag* and *saga* are just as accurate as the other solvers.

```
liblinear 0.960
newton-cg 0.962
lbfgs 0.962
sag 0.962
saga 0.962
```

Now let's look at an example with three classes.

## Multi-class solver example

I evaluated the logistic regression solvers in a multi-class classification problem with Scikit-learn's wine dataset. The dataset contains 178 samples and 13 numeric features. The goal is to predict the type of grapes used to make the wine from the chemical features of the wine.

```
solver_list = ['liblinear', 'newton-cg', 'lbfgs', 'sag', 'saga']
parameters = dict(solver=solver_list)
lr = LogisticRegression(random_state=34, multi_class="auto",
n_jobs=-1, C=1)
clf = GridSearchCV(lr, parameters, cv=5)
clf.fit(X_train, y_train)
scores = clf.cv_results_['mean_test_score']

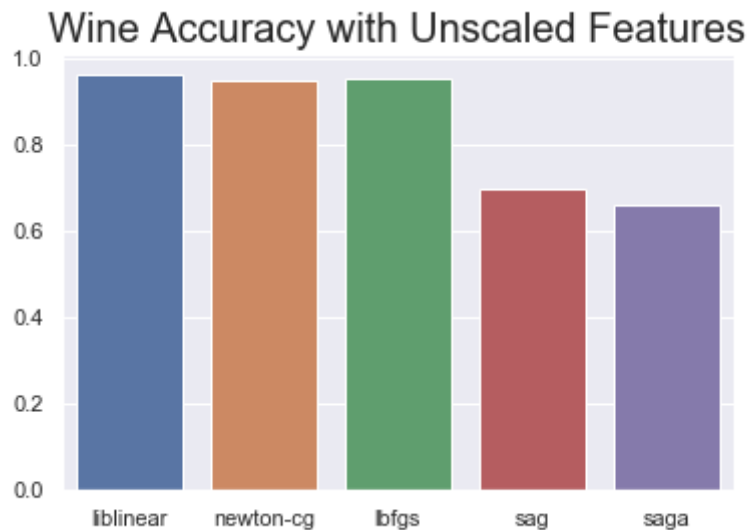
for score, solver, in zip(scores, solver_list):
    print(f"{solver}: {score:.3f}")
```

Scikit-learn gives a warning that the *sag* and *saga* models did not converge. In other words, they never arrived at a minimum point. Unsurprisingly, the results aren't so great for those solvers.

```
liblinear: 0.962
newton-cg: 0.947
```

```
lbfgs: 0.955  
sag: 0.699  
saga: 0.662
```

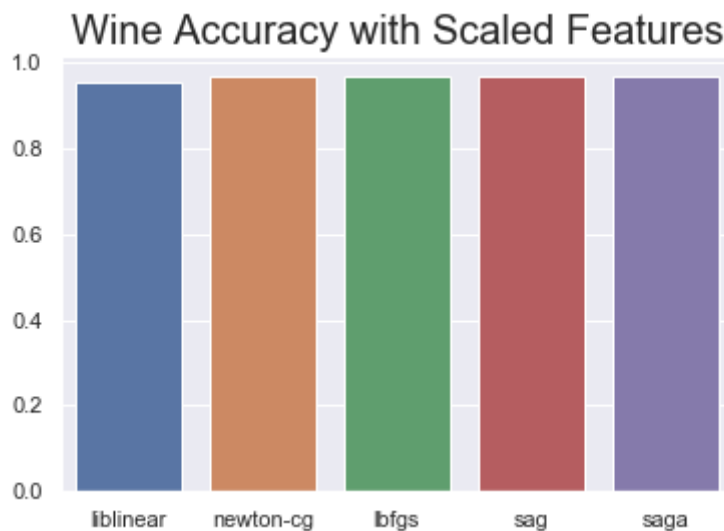
Let's make a little bar chart using the Seaborn library to show the scores.



sag and saga lagging show lower accuracy

After scaling the features between 0 and 1, then *sag* and *saga* reach the same mean accuracy scores as the other models.

```
liblinear: 0.955  
newton-cg: 0.970  
lbfgs: 0.970  
sag: 0.970  
saga: 0.970
```



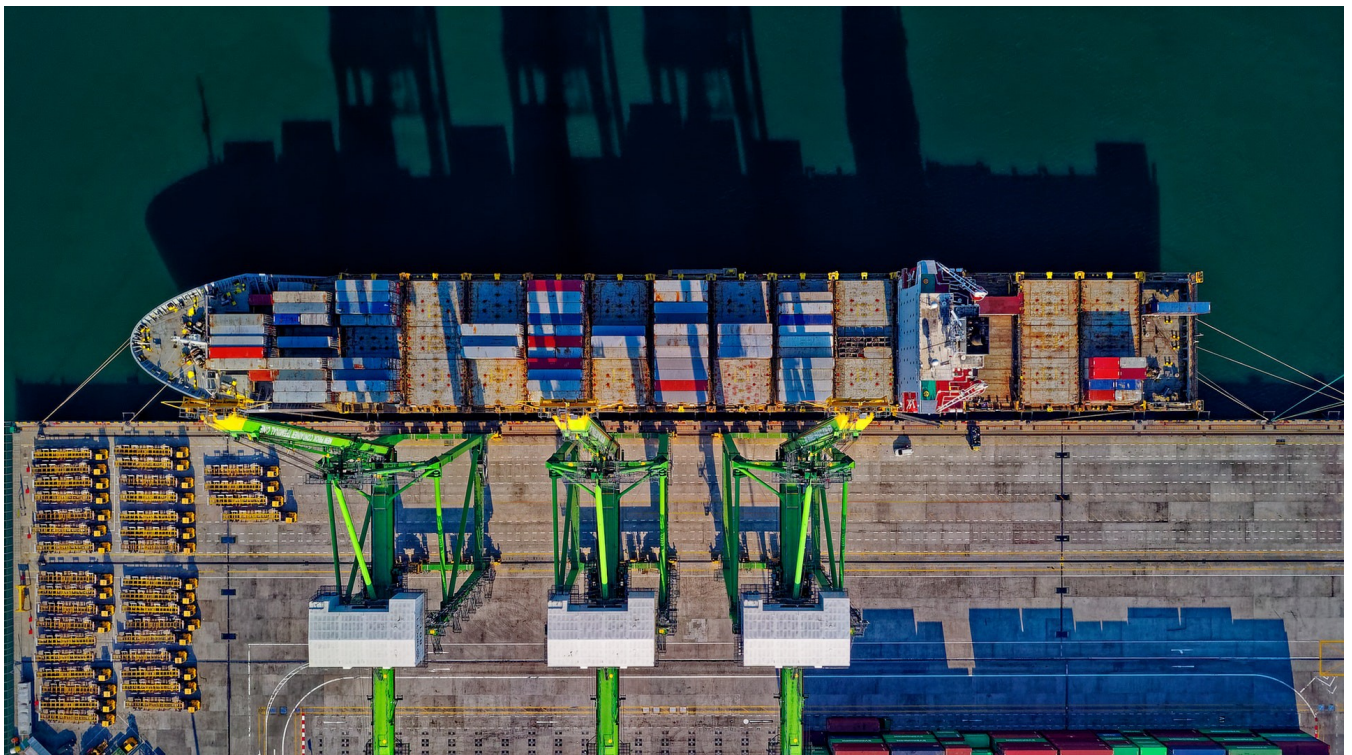
Looking better for sag and saga

Note the caveat that both of these examples are with small datasets. Also, we're not looking at memory and speed requirements in these examples.

Bottom line: the forthcoming default *lbfgs* solver is a good first choice for most cases. If you're dealing with a large dataset or want to apply L1 regularization, I suggest you start with *saga*. Remember that *saga* needs the features to be on a similar scale.

Do you have a use case for *newton-cg* or *sag*? If so, please share in the comments. 

Next, I'll demystify key parameter options for LogisticRegression in Scikit-learn.



Logistics



## Parameters

The Scikit-learn LogisticRegression class can take the following arguments.

```
penalty, dual, tol, C, fit_intercept, intercept_scaling, class_weight,
random_state, solver, max_iter, verbose, warm_start, n_jobs, l1_ratio
```

I won't include all of the parameters below, just excerpts from those parameters most likely to be valuable to most folks. See the [docs](#) for those that are omitted. I've added additional information in *italics*.

**C** — float, optional, default = 1. Smaller values have more regularization. Inverse of regularization strength. *Must be positive value. Usually search logarithmically: [.001, .01, .1, 1, 10, 100, 1000]*

**random\_state** : int, RandomState instance or None, optional (default=None) *Note that you must set the random state here for reproducibility.*

**solver** {'newton-cg', 'lbfgs', 'liblinear', 'sag', 'saga'}, optional (default='liblinear'). *See the chart above for more info.*

**Changed in version 0.20: Default will change from 'liblinear' to 'lbfgs' in 0.22.**

**multi\_class** : str, {'ovr', 'multinomial', 'auto'}, optional (default='ovr') If the option chosen is 'ovr', then a binary problem is fit for each label. For 'multinomial' the loss minimised is the multinomial loss fit across the entire probability distribution, even when the data is binary. 'multinomial' is unavailable when solver='liblinear'. 'auto' selects 'ovr' if the data is binary, or if solver='liblinear', and otherwise selects 'multinomial'.

**Changed in version 0.20: Default will change from 'ovr' to 'auto' in 0.22. ovr stands for one vs. rest. See further discussion below.**

**l1\_ratio** : float or None, optional (default=None) The Elastic-Net mixing parameter, with  $0 \leq \text{l1\_ratio} \leq 1$ . Only used if penalty='elasticnet'. Setting 'l1\_ratio=0 is equivalent to using penalty='l2', while setting l1\_ratio=1 is equivalent to using penalty='l1'. For  $0 < \text{l1\_ratio} < 1$ , the penalty is a combination of L1 and L2. *Only for saga.*

*Commentary:* If you have a multiclass problem, then setting `multi-class` to `auto` will use the multinomial option every time it's available. That's the most theoretically sound choice. `auto` will soon be the default.

Use `l1_ratio` if you want to use some L1 regularization with the *saga* solver. Note that like the ElasticNet linear regression option, you can use a mix of L1 and L2 penalization.

Also note that an L2 regularization of `C=1` is applied by default. This default regularization makes models more robust to multicollinearity, but at the expense of less interpretability (hat tip to Andreas Mueller).

After fitting the model the attributes are: `classes_`, `coef_`, `intercept_`, and `n_iter`. `coef_` contains an array of the feature weights.

## Logistic Regression FAQ

Now let's address those nagging questions you might have about Logistic Regression in Scikit-learn.

### Can I use LogisticRegression for a multilabel problem — meaning one output can be a member of multiple classes at once?

Nope. Sorry, if you need that, find another classification algorithm [here](#).

### Which kind of regularization should I use?

Regularization shifts your model toward the bias side of things in the bias/variance tradeoff. Regularization makes for a more generalizable logistic regression model, especially in cases with few data points. You'll probably want to hyperparameter search over the regularization parameter *C*.

If you want to do some dimensionality reduction through regularization, use L1 regularization. L1 regularization is Manhattan or Taxicab regularization. L2 regularization is Euclidian regularization and generally performs better in generalized linear regression problems.

You must use the *saga* solver if you want to apply a mix of L1 and L2 regularization. The *liblinear* solver requires you to have regularization. However, you could just make *C* such as a large value that it had a very, very small regularization penalty. Again, *C* is currently set to 1 by default.

## Should I scale the features?



Scale

If using *sag* and *saga* solvers, make sure the features are on a similar scale. We saw the importance of this above. Andreas Mueller, in private correspondence, also mentioned that he found convergence issues on unscaled data with *lbfgs*, although it was more robust than *sag* and *saga*.

Bottom line: to be safe, scale your data.

## Should I remove outliers?

Probably. Removing outliers will generally improve model performance. Standardizing the inputs would also reduce outliers' effects.

RobustScaler can scale features and you can avoid dropping outliers. See my article discussing scaling and standardizing [here](#).

## Which other assumptions really matter?

Observations should be independent of each other.

## Should I transform my features using polynomials and interactions?

Just as in linear regression, you can use higher order polynomials and interactions. This transformation allows your model to learn a more complex decision boundary. Then, you aren't limited to a linear decision boundary. However, overfitting becomes a risk and interpreting feature importances gets trickier. It might also be more difficult for the solver to find the global minimum.



Transformation

## Should I do dimensionality reduction if there are lots of features?

Maybe. Principal Components Analysis is a nice choice if interpretability isn't vital. Recursive Feature Elimination can help you remove the least important features. Alternatively, L1 regularization can drive less important feature weights to zero if you are using the *saga* solver.

## Is multicollinearity in my features a problem?

It is for interpretation of the feature importances. You can't rely on the model weights to be meaningful when there is high correlation between the variables. Credit for affecting the outcome variable might go to just one of the correlated features.

There are many ways to test for multicollinearity. See [Kraha et al. \(2012\) here](#).



One popular option is to check the Variance Inflation Factor (VIF). A VIF cutoff around 5 to 10 is common, but there's a [lively debate](#) as to what an appropriate VIF cutoff should be.

You can compute the VIF by taking the correlation matrix, inverting it, and taking the values on the diagonal for each feature.

The correlation coefficients alone are not sufficient to determine problematic multicollinearity with multiple features.

If the sample size is small, getting more data might be most helpful for removing multicollinearity.

## When should I use `LogisticRegressionCV`?

`LogisticRegressionCV` is the Scikit-learn algorithm you want if you have a lot of data and want to speed up your calculations while doing cross-validation to tune your hyperparameters.

## Wrap

Now you know what to do when you see the `LogisticRegression` solver warning — and better yet, how to avoid it in the first place. No more sweat! 😊

I suggest you use the upcoming default `lbfgs` solver for most cases. If you have a lot of data or need L1 regularization, try `saga`. Make sure you scale your features if you're using `saga`.

I hope you found this discussion of logistic regression helpful. If you did, please share it on your favorite social media so other people can find it, too. 👍

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