

Data Analysis and Machine Learning: Logistic Regression and Gradient Methods

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Logistic Regression

In linear regression our main interest was centered on learning the coefficients of a functional fit (say a polynomial) in order to be able to predict the response of a continuous variable on some unseen data. The fit to the continuous variable y_i is based on some independent variables \hat{x}_i . Linear regression resulted in analytical expressions for standard ordinary Least Squares or Ridge regression (in terms of matrices to invert) for several quantities, ranging from the variance and thereby the confidence intervals of the parameters $\hat{\beta}$ to the mean squared error. If we can invert the product of the design matrices, linear regression gives then a simple recipe for fitting our data.

Logistic Regression and Classification Problems

Classification problems, however, are concerned with outcomes taking the form of discrete variables (i.e. categories). We may for example, on the basis of DNA sequencing for a number of patients, like to find out which mutations are important for a certain disease; or based on scans of various patients' brains, figure out if there is a tumor or not; or given a specific physical system, we'd like to identify its state, say whether it is an ordered or disordered system (typical situation in solid state physics); or classify the status of a patient, whether she/he has a stroke or not and many other similar situations.

The most common situation we encounter when we apply logistic regression is that of two possible outcomes, normally denoted as a binary outcome, true or false, positive or negative, success or failure etc.

Optimization and Deep learning

Logistic regression will also serve as our stepping stone towards neural network algorithms and supervised deep learning. For logistic learning, the minimization of the cost function leads to a non-linear equation in the parameters $\hat{\beta}$. The optimization of the problem calls therefore for minimization algorithms. This forms the bottle neck of all machine learning algorithms, namely how to find reliable minima of a multi-variable function. This leads us to the family of gradient descent methods. The latter are the working horses of basically all modern machine learning algorithms.

We note also that many of the topics discussed here on logistic regression are also commonly used in modern supervised Deep Learning models, as we will see later.

Basics

We consider the case where the dependent variables, also called the responses or the outcomes, y_i are discrete and only take values from $k = 0, \dots, K - 1$ (i.e. K classes).

The goal is to predict the output classes from the design matrix $\hat{X} \in \mathbb{R}^{n \times p}$ made of n samples, each of which carries p features or predictors. The primary goal is to identify the classes to which new unseen samples belong.

Let us specialize to the case of two classes only, with outputs $y_i = 0$ and $y_i = 1$. Our outcomes could represent the status of a credit card user that could default or not on her/his credit card debt. That is

$$y_i = \begin{bmatrix} 0 & \text{no} \\ 1 & \text{yes} \end{bmatrix}.$$

Linear classifier

Before moving to the logistic model, let us try to use our linear regression model to classify these two outcomes. We could for example fit a linear model to the default case if $y_i > 0.5$ and the no default case $y_i \leq 0.5$.

We would then have our weighted linear combination, namely

$$\hat{y} = \hat{X}^T \hat{\beta} + \hat{\epsilon}, \quad (1)$$

where \hat{y} is a vector representing the possible outcomes, \hat{X} is our $n \times p$ design matrix and $\hat{\beta}$ represents our estimators/predictors.

Some selected properties

The main problem with our function is that it takes values on the entire real axis. In the case of logistic regression, however, the labels y_i are discrete variables. A typical example is the credit card data discussed earlier, where we can set the state of defaulting the debt to $y_i = 1$ and not to $y_i = 0$ for one the persons in the data set (see the full example below).

One simple way to get a discrete output is to have sign functions that map the output of a linear regressor to values $\{0, 1\}$, $f(s_i) = \text{sign}(s_i) = 1$ if $s_i \geq 0$ and 0 if otherwise. We will encounter this model in our first demonstration of neural networks. Historically it is called the “perceptron” model in the machine learning literature. This model is extremely simple. However, in many cases it is more favorable to use a “soft” classifier that outputs the probability of a given category. This leads us to the logistic function.

The logistic function

The perceptron is an example of a “hard classification” model. We will encounter this model when we discuss neural networks as well. Each datapoint is deterministically assigned to a category (i.e $y_i = 0$ or $y_i = 1$). In many cases, it is favorable to have a “soft” classifier that outputs the probability of a given category rather than a single value. For example, given x_i , the classifier outputs the probability of being in a category k . Logistic regression is the most common example of a so-called soft classifier. In logistic regression, the probability that a data point x_i belongs to a category $y_i = \{0, 1\}$ is given by the so-called logit function (or Sigmoid) which is meant to represent the likelihood for a given event,

$$p(t) = \frac{1}{1 + \exp(-t)} = \frac{\exp t}{1 + \exp t}.$$

Note that $1 - p(t) = p(-t)$.

Examples of likelihood functions used in logistic regression and neural networks

The following code plots the logistic function, the step function and other functions we will encounter from here and on.

Two parameters

We assume now that we have two classes with y_i either 0 or 1. Furthermore we assume also that we have only two parameters β in our fitting of the Sigmoid function, that is we define probabilities

$$p(y_i = 1|x_i, \hat{\beta}) = \frac{\exp(\beta_0 + \beta_1 x_i)}{1 + \exp(\beta_0 + \beta_1 x_i)},$$

$$p(y_i = 0|x_i, \hat{\beta}) = 1 - p(y_i = 1|x_i, \hat{\beta}),$$

where $\hat{\beta}$ are the weights we wish to extract from data, in our case β_0 and β_1 .

Note that we used

$$p(y_i = 0|x_i, \hat{\beta}) = 1 - p(y_i = 1|x_i, \hat{\beta}).$$

Maximum likelihood

In order to define the total likelihood for all possible outcomes from a dataset $\mathcal{D} = \{(y_i, x_i)\}$, with the binary labels $y_i \in \{0, 1\}$ and where the data points are drawn independently, we use the so-called [Maximum Likelihood Estimation](#) (MLE) principle. We aim thus at maximizing the probability of seeing the observed data. We can then approximate the likelihood in terms of the product of the individual probabilities of a specific outcome y_i , that is

$$P(\mathcal{D}|\hat{\beta}) = \prod_{i=1}^n \left[p(y_i = 1|x_i, \hat{\beta}) \right]^{y_i} \left[1 - p(y_i = 1|x_i, \hat{\beta}) \right]^{1-y_i}$$

from which we obtain the log-likelihood and our **cost/loss** function

$$\mathcal{C}(\hat{\beta}) = \sum_{i=1}^n \left(y_i \log p(y_i = 1|x_i, \hat{\beta}) + (1 - y_i) \log \left[1 - p(y_i = 1|x_i, \hat{\beta}) \right] \right).$$

The cost function rewritten

Reordering the logarithms, we can rewrite the **cost/loss** function as

$$\mathcal{C}(\hat{\beta}) = \sum_{i=1}^n (y_i(\beta_0 + \beta_1 x_i) - \log(1 + \exp(\beta_0 + \beta_1 x_i))).$$

The maximum likelihood estimator is defined as the set of parameters that maximize the log-likelihood where we maximize with respect to β . Since the cost (error) function is just the negative log-likelihood, for logistic regression we have that

$$\mathcal{C}(\hat{\beta}) = - \sum_{i=1}^n (y_i(\beta_0 + \beta_1 x_i) - \log(1 + \exp(\beta_0 + \beta_1 x_i))).$$

This equation is known in statistics as the **cross entropy**. Finally, we note that just as in linear regression, in practice we often supplement the cross-entropy with additional regularization terms, usually L_1 and L_2 regularization as we did for Ridge and Lasso regression.

Minimizing the cross entropy

The cross entropy is a convex function of the weights $\hat{\beta}$ and, therefore, any local minimizer is a global minimizer.

Minimizing this cost function with respect to the two parameters β_0 and β_1 we obtain

$$\frac{\partial \mathcal{C}(\hat{\beta})}{\partial \beta_0} = - \sum_{i=1}^n \left(y_i - \frac{\exp(\beta_0 + \beta_1 x_i)}{1 + \exp(\beta_0 + \beta_1 x_i)} \right),$$

and

$$\frac{\partial \mathcal{C}(\hat{\beta})}{\partial \beta_1} = - \sum_{i=1}^n \left(y_i x_i - x_i \frac{\exp(\beta_0 + \beta_1 x_i)}{1 + \exp(\beta_0 + \beta_1 x_i)} \right).$$

A more compact expression

Let us now define a vector \hat{y} with n elements y_i , an $n \times p$ matrix \hat{X} which contains the x_i values and a vector \hat{p} of fitted probabilities $p(y_i|x_i, \hat{\beta})$. We can rewrite in a more compact form the first derivative of cost function as

$$\frac{\partial \mathcal{C}(\hat{\beta})}{\partial \hat{\beta}} = -\hat{X}^T (\hat{y} - \hat{p}).$$

If we in addition define a diagonal matrix \hat{W} with elements $p(y_i|x_i, \hat{\beta})(1 - p(y_i|x_i, \hat{\beta}))$, we can obtain a compact expression of the second derivative as

$$\frac{\partial^2 \mathcal{C}(\hat{\beta})}{\partial \hat{\beta} \partial \hat{\beta}^T} = \hat{X}^T \hat{W} \hat{X}.$$

Extending to more predictors

Within a binary classification problem, we can easily expand our model to include multiple predictors. Our ratio between likelihoods is then with p predictors

$$\log \frac{p(\hat{\beta}\hat{x})}{1 - p(\hat{\beta}\hat{x})} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p.$$

Here we defined $\hat{x} = [1, x_1, x_2, \dots, x_p]$ and $\hat{\beta} = [\beta_0, \beta_1, \dots, \beta_p]$ leading to

$$p(\hat{\beta}\hat{x}) = \frac{\exp(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p)}{1 + \exp(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p)}.$$

Including more classes

Till now we have mainly focused on two classes, the so-called binary system. Suppose we wish to extend to K classes. Let us for the sake of simplicity assume we have only two predictors. We have then following model

$$\begin{aligned} \log \frac{p(C=1|x)}{p(K|x)} &= \beta_{10} + \beta_{11} x_1, \\ \log \frac{p(C=2|x)}{p(K|x)} &= \beta_{20} + \beta_{21} x_1, \end{aligned}$$

and so on till the class $C = K - 1$ class

$$\log \frac{p(C=K-1|x)}{p(K|x)} = \beta_{(K-1)0} + \beta_{(K-1)1} x_1,$$

and the model is specified in term of $K - 1$ so-called log-odds or **logit** transformations.

More classes

In our discussion of neural networks we will encounter the above again in terms of a slightly modified function, the so-called **Softmax** function.

The softmax function is used in various multiclass classification methods, such as multinomial logistic regression (also known as softmax regression), multiclass linear discriminant analysis, naive Bayes classifiers, and artificial neural networks. Specifically, in multinomial logistic regression and linear discriminant analysis, the input to the function is the result of K distinct linear functions, and the predicted probability for the k -th class given a sample vector \hat{x} and a weighting vector $\hat{\beta}$ is (with two predictors):

$$p(C = k|\mathbf{x}) = \frac{\exp(\beta_{k0} + \beta_{k1}x_1)}{1 + \sum_{l=1}^{K-1} \exp(\beta_{l0} + \beta_{l1}x_1)}.$$

It is easy to extend to more predictors. The final class is

$$p(C = K|\mathbf{x}) = \frac{1}{1 + \sum_{l=1}^{K-1} \exp(\beta_{l0} + \beta_{l1}x_1)},$$

and they sum to one. Our earlier discussions were all specialized to the case with two classes only. It is easy to see from the above that what we derived earlier is compatible with these equations.

To find the optimal parameters we would typically use a gradient descent method. Newton's method and gradient descent methods are discussed in the material on [optimization methods](#).

Preprocessing our data

We discuss here how to preprocess our data. Till now and in connection with our previous examples we have not met so many cases where we are too sensitive to the scaling of our data. Normally the data may need a rescaling and/or may be sensitive to extreme values. Scaling the data renders our inputs much more suitable for the algorithms we want to employ.

Scikit-Learn has several functions which allow us to rescale the data, normally resulting in much better results in terms of various accuracy scores. The **StandardScaler** function in **Scikit-Learn** ensures that for each feature/predictor we study the mean value is zero and the variance is one (every column in the design/feature matrix). This scaling has the drawback that it does not ensure that we have a particular maximum or minimum in our data set. Another function included in **Scikit-Learn** is the **MinMaxScaler** which ensures that all features are exactly between 0 and 1. The

More preprocessing

The **Normalizer** scales each data point such that the feature vector has a euclidean length of one. In other words, it projects a data point on the circle (or sphere in the case of higher dimensions) with a radius of 1. This means

every data point is scaled by a different number (by the inverse of it's length). This normalization is often used when only the direction (or angle) of the data matters, not the length of the feature vector.

The **RobustScaler** works similarly to the **StandardScaler** in that it ensures statistical properties for each feature that guarantee that they are on the same scale. However, the **RobustScaler** uses the median and quartiles, instead of mean and variance. This makes the **RobustScaler** ignore data points that are very different from the rest (like measurement errors). These odd data points are also called outliers, and might often lead to trouble for other scaling techniques.

Simple preprocessing examples, breast cancer data and classification

We show here how we can use a simple regression case on the breast cancer data using logistic regression as algorithm for classification.

Covariance and Correlation

In addition to the plot of the features, we study now also the covariance (and the correlation matrix). We use also **Pandas** to compute the correlation matrix.

In the above example we note two things. In the first plot we display the overlap of benign and malignant tumors as functions of the various features in the Wisconsin breast cancer data set. We see that for some of the features we can distinguish clearly the benign and malignant cases while for other features we cannot. This can point to us which features may be of greater interest when we wish to classify a benign or not benign tumour.

In the second figure we have computed the so-called correlation matrix, which in our case with thirty features becomes a 30×30 matrix.

We constructed this matrix using **pandas** via the statements and then

Diagonalizing this matrix we can in turn say something about which features are of relevance and which are not. This leads us to the classical Principal Component Analysis (PCA) theorem with applications. This topic is covered in the PCA material and additional topics on dimensionality reduction.

Optimization, the central part of any Machine Learning algorithm

Almost every problem in machine learning and data science starts with a dataset X , a model $g(\beta)$, which is a function of the parameters β and a cost function $C(X, g(\beta))$ that allows us to judge how well the model $g(\beta)$ explains the observations X . The model is fit by finding the values of β that minimize the cost function. Ideally we would be able to solve for β analytically, however this is not possible in general and we must use some approximative/numerical method to compute the minimum.

Revisiting our Logistic Regression case

In our discussion on Logistic Regression we studied the case of two classes, with y_i either 0 or 1. Furthermore we assumed also that we have only two parameters β in our fitting, that is we defined probabilities

$$p(y_i = 1|x_i, \hat{\beta}) = \frac{\exp(\beta_0 + \beta_1 x_i)}{1 + \exp(\beta_0 + \beta_1 x_i)},$$
$$p(y_i = 0|x_i, \hat{\beta}) = 1 - p(y_i = 1|x_i, \hat{\beta}),$$

where $\hat{\beta}$ are the weights we wish to extract from data, in our case β_0 and β_1 .

The equations to solve

Our compact equations used a definition of a vector \hat{y} with n elements y_i , an $n \times p$ matrix \hat{X} which contains the x_i values and a vector \hat{p} of fitted probabilities $p(y_i|x_i, \hat{\beta})$. We rewrote in a more compact form the first derivative of the cost function as

$$\frac{\partial \mathcal{C}(\hat{\beta})}{\partial \hat{\beta}} = -\hat{X}^T (\hat{y} - \hat{p}).$$

If we in addition define a diagonal matrix \hat{W} with elements $p(y_i|x_i, \hat{\beta})(1 - p(y_i|x_i, \hat{\beta}))$, we can obtain a compact expression of the second derivative as

$$\frac{\partial^2 \mathcal{C}(\hat{\beta})}{\partial \hat{\beta} \partial \hat{\beta}^T} = \hat{X}^T \hat{W} \hat{X}.$$

This defines what is called the Hessian matrix.

Solving using Newton-Raphson's method

If we can set up these equations, Newton-Raphson's iterative method is normally the method of choice. It requires however that we can compute in an efficient way the matrices that define the first and second derivatives.

Our iterative scheme is then given by

$$\hat{\beta}^{\text{new}} = \hat{\beta}^{\text{old}} - \left(\frac{\partial^2 \mathcal{C}(\hat{\beta})}{\partial \hat{\beta} \partial \hat{\beta}^T} \right)_{\hat{\beta}^{\text{old}}}^{-1} \times \left(\frac{\partial \mathcal{C}(\hat{\beta})}{\partial \hat{\beta}} \right)_{\hat{\beta}^{\text{old}}},$$

or in matrix form as

$$\hat{\beta}^{\text{new}} = \hat{\beta}^{\text{old}} - \left(\hat{X}^T \hat{W} \hat{X} \right)^{-1} \times \left(-\hat{X}^T (\hat{y} - \hat{p}) \right)_{\hat{\beta}^{\text{old}}}.$$

The right-hand side is computed with the old values of β .

If we can compute these matrices, in particular the Hessian, the above is often the easiest method to implement.

Brief reminder on Newton-Raphson's method

Let us quickly remind ourselves how we derive the above method.

Perhaps the most celebrated of all one-dimensional root-finding routines is Newton's method, also called the Newton-Raphson method. This method requires the evaluation of both the function f and its derivative f' at arbitrary points. If you can only calculate the derivative numerically and/or your function is not of the smooth type, we normally discourage the use of this method.

The equations

The Newton-Raphson formula consists geometrically of extending the tangent line at a current point until it crosses zero, then setting the next guess to the abscissa of that zero-crossing. The mathematics behind this method is rather simple. Employing a Taylor expansion for x sufficiently close to the solution s , we have

$$f(s) = 0 = f(x) + (s - x)f'(x) + \frac{(s - x)^2}{2}f''(x) + \dots$$

For small enough values of the function and for well-behaved functions, the terms beyond linear are unimportant, hence we obtain

$$f(x) + (s - x)f'(x) \approx 0,$$

yielding

$$s \approx x - \frac{f(x)}{f'(x)}.$$

Having in mind an iterative procedure, it is natural to start iterating with

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}.$$

Simple geometric interpretation

The above is Newton-Raphson's method. It has a simple geometric interpretation, namely x_{n+1} is the point where the tangent from $(x_n, f(x_n))$ crosses the x -axis. Close to the solution, Newton-Raphson converges fast to the desired result. However, if we are far from a root, where the higher-order terms in the series are important, the Newton-Raphson formula can give grossly inaccurate results. For instance, the initial guess for the root might be so far from the true root as to let the search interval include a local maximum or minimum of the function. If an iteration places a trial guess near such a local extremum, so that the first derivative nearly vanishes, then Newton-Raphson may fail totally

Extending to more than one variable

Newton's method can be generalized to systems of several non-linear equations and variables. Consider the case with two equations

$$\begin{aligned} f_1(x_1, x_2) &= 0 \\ f_2(x_1, x_2) &= 0, \end{aligned}$$

which we Taylor expand to obtain

$$\begin{aligned} 0 = f_1(x_1 + h_1, x_2 + h_2) &= f_1(x_1, x_2) + h_1 \partial f_1 / \partial x_1 + h_2 \partial f_1 / \partial x_2 + \dots \\ 0 = f_2(x_1 + h_1, x_2 + h_2) &= f_2(x_1, x_2) + h_1 \partial f_2 / \partial x_1 + h_2 \partial f_2 / \partial x_2 + \dots \end{aligned}$$

Defining the Jacobian matrix $\hat{\mathbf{J}}$ we have

$$\hat{\mathbf{J}} = \begin{pmatrix} \partial f_1 / \partial x_1 & \partial f_1 / \partial x_2 \\ \partial f_2 / \partial x_1 & \partial f_2 / \partial x_2 \end{pmatrix},$$

we can rephrase Newton's method as

$$\begin{pmatrix} x_1^{n+1} \\ x_2^{n+1} \end{pmatrix} = \begin{pmatrix} x_1^n \\ x_2^n \end{pmatrix} + \begin{pmatrix} h_1^n \\ h_2^n \end{pmatrix},$$

where we have defined

$$\begin{pmatrix} h_1^n \\ h_2^n \end{pmatrix} = -\hat{\mathbf{J}}^{-1} \begin{pmatrix} f_1(x_1^n, x_2^n) \\ f_2(x_1^n, x_2^n) \end{pmatrix}.$$

We need thus to compute the inverse of the Jacobian matrix and it is to understand that difficulties may arise in case $\hat{\mathbf{J}}$ is nearly singular.

It is rather straightforward to extend the above scheme to systems of more than two non-linear equations. In our case, the Jacobian matrix is given by the Hessian that represents the second derivative of cost function.

Steepest descent

The basic idea of gradient descent is that a function $F(\mathbf{x})$, $\mathbf{x} \equiv (x_1, \dots, x_n)$, decreases fastest if one goes from \mathbf{x} in the direction of the negative gradient $-\nabla F(\mathbf{x})$.

It can be shown that if

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \gamma_k \nabla F(\mathbf{x}_k),$$

with $\gamma_k > 0$.

For γ_k small enough, then $F(\mathbf{x}_{k+1}) \leq F(\mathbf{x}_k)$. This means that for a sufficiently small γ_k we are always moving towards smaller function values, i.e a minimum.

More on Steepest descent

The previous observation is the basis of the method of steepest descent, which is also referred to as just gradient descent (GD). One starts with an initial guess \mathbf{x}_0 for a minimum of F and computes new approximations according to

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \gamma_k \nabla F(\mathbf{x}_k), \quad k \geq 0.$$

The parameter γ_k is often referred to as the step length or the learning rate within the context of Machine Learning.

The ideal

Ideally the sequence $\{\mathbf{x}_k\}_{k=0}$ converges to a global minimum of the function F . In general we do not know if we are in a global or local minimum. In the special case when F is a convex function, all local minima are also global minima, so in this case gradient descent can converge to the global solution. The advantage of this scheme is that it is conceptually simple and straightforward to implement. However the method in this form has some severe limitations:

In machine learning we are often faced with non-convex high dimensional cost functions with many local minima. Since GD is deterministic we will get stuck in a local minimum, if the method converges, unless we have a very good initial guess. This also implies that the scheme is sensitive to the chosen initial condition.

Note that the gradient is a function of $\mathbf{x} = (x_1, \dots, x_n)$ which makes it expensive to compute numerically.

The sensitiveness of the gradient descent

The gradient descent method is sensitive to the choice of learning rate γ_k . This is due to the fact that we are only guaranteed that $F(\mathbf{x}_{k+1}) \leq F(\mathbf{x}_k)$ for sufficiently small γ_k . The problem is to determine an optimal learning rate. If the learning rate is chosen too small the method will take a long time to converge and if it is too large we can experience erratic behavior.

Many of these shortcomings can be alleviated by introducing randomness. One such method is that of Stochastic Gradient Descent (SGD), see below.

Convex functions

Ideally we want our cost/loss function to be convex(concave).

First we give the definition of a convex set: A set C in \mathbb{R}^n is said to be convex if, for all x and y in C and all $t \in (0, 1)$, the point $(1 - t)x + ty$ also belongs to C . Geometrically this means that every point on the line segment connecting x and y is in C as discussed below.

The convex subsets of \mathbb{R} are the intervals of \mathbb{R} . Examples of convex sets of \mathbb{R}^2 are the regular polygons (triangles, rectangles, pentagons, etc...).

Convex function

Convex function: Let $X \subset \mathbb{R}^n$ be a convex set. Assume that the function $f : X \rightarrow \mathbb{R}$ is continuous, then f is said to be convex if

$$f(tx_1 + (1-t)x_2) \leq tf(x_1) + (1-t)f(x_2)$$

for all $x_1, x_2 \in X$ and for all $t \in [0, 1]$. If \leq is replaced with a strict inequality in the definition, we demand $x_1 \neq x_2$ and $t \in (0, 1)$ then f is said to be strictly convex. For a single variable function, convexity means that if you draw a straight line connecting $f(x_1)$ and $f(x_2)$, the value of the function on the interval $[x_1, x_2]$ is always below the line as illustrated below.

Conditions on convex functions

In the following we state first and second-order conditions which ensures convexity of a function f . We write D_f to denote the domain of f , i.e the subset of \mathbb{R}^n where f is defined. For more details and proofs we refer to: [S. Boyd and L. Vandenberghe. Convex Optimization. Cambridge University Press.](#)

First order condition. Suppose f is differentiable (i.e $\nabla f(x)$ is well defined for all x in the domain of f). Then f is convex if and only if D_f is a convex set and

$$f(y) \geq f(x) + \nabla f(x)^T(y - x)$$

holds for all $x, y \in D_f$. This condition means that for a convex function the first order Taylor expansion (right hand side above) at any point a global under estimator of the function. To convince yourself you can make a drawing of $f(x) = x^2 + 1$ and draw the tangent line to $f(x)$ and note that it is always below the graph.

Second order condition. Assume that f is twice differentiable, i.e the Hessian matrix exists at each point in D_f . Then f is convex if and only if D_f is a convex set and its Hessian is positive semi-definite for all $x \in D_f$. For a single-variable function this reduces to $f''(x) \geq 0$. Geometrically this means that f has nonnegative curvature everywhere.

This condition is particularly useful since it gives us an procedure for determining if the function under consideration is convex, apart from using the definition.

More on convex functions

The next result is of great importance to us and the reason why we are going on about convex functions. In machine learning we frequently have to minimize a loss/cost function in order to find the best parameters for the model we are considering.

Ideally we want the global minimum (for high-dimensional models it is hard to know if we have local or global minimum). However, if the cost/loss function is convex the following result provides invaluable information:

Any minimum is global for convex functions. Consider the problem of finding $x \in \mathbb{R}^n$ such that $f(x)$ is minimal, where f is convex and differentiable. Then, any point x^* that satisfies $\nabla f(x^*) = 0$ is a global minimum.

This result means that if we know that the cost/loss function is convex and we are able to find a minimum, we are guaranteed that it is a global minimum.

Some simple problems

1. Show that $f(x) = x^2$ is convex for $x \in \mathbb{R}$ using the definition of convexity. Hint: If you re-write the definition, f is convex if the following holds for all $x, y \in D_f$ and any $\lambda \in [0, 1]$ $\lambda f(x) + (1 - \lambda)f(y) - f(\lambda x + (1 - \lambda)y) \geq 0$.
2. Using the second order condition show that the following functions are convex on the specified domain.
 - $f(x) = e^x$ is convex for $x \in \mathbb{R}$.
 - $g(x) = -\ln(x)$ is convex for $x \in (0, \infty)$.
3. Let $f(x) = x^2$ and $g(x) = e^x$. Show that $f(g(x))$ and $g(f(x))$ is convex for $x \in \mathbb{R}$. Also show that if $f(x)$ is any convex function then $h(x) = e^{f(x)}$ is convex.
4. A norm is any function that satisfy the following properties
 - $f(\alpha x) = |\alpha|f(x)$ for all $\alpha \in \mathbb{R}$.
 - $f(x + y) \leq f(x) + f(y)$
 - $f(x) \leq 0$ for all $x \in \mathbb{R}^n$ with equality if and only if $x = 0$

Using the definition of convexity, try to show that a function satisfying the properties above is convex (the third condition is not needed to show this).

Revisiting our first homework

We will use linear regression as a case study for the gradient descent methods. Linear regression is a great test case for the gradient descent methods discussed in the lectures since it has several desirable properties such as:

1. An analytical solution (recall homework set 1).
2. The gradient can be computed analytically.
3. The cost function is convex which guarantees that gradient descent converges for small enough learning rates

We revisit the example from homework set 1 where we had

$$y_i = 5x_i^2 + 0.1\xi_i, \quad i = 1, \dots, 100$$

with $x_i \in [0, 1]$ chosen randomly with a uniform distribution. Additionally ξ_i represents stochastic noise chosen according to a normal distribution $\mathcal{N}(\iota, \infty)$. The linear regression model is given by

$$h_\beta(x) = \hat{y} = \beta_0 + \beta_1 x,$$

such that

$$\hat{y}_i = \beta_0 + \beta_1 x_i.$$

Gradient descent example

Let $\mathbf{y} = (y_1, \dots, y_n)^T$, $\hat{\mathbf{y}} = (\hat{y}_1, \dots, \hat{y}_n)^T$ and $\beta = (\beta_0, \beta_1)^T$

It is convenient to write $\hat{\mathbf{y}} = X\beta$ where $X \in \mathbb{R}^{100 \times 2}$ is the design matrix given by

$$X \equiv \begin{bmatrix} 1 & \text{amp;} x_1 \\ \vdots & \text{amp;} \vdots \\ 1 & \text{amp;} x_{100} & \text{amp;} \end{bmatrix}.$$

The loss function is given by

$$C(\beta) = \|X\beta - \mathbf{y}\|^2 = \|X\beta\|^2 - 2\mathbf{y}^T X\beta + \|\mathbf{y}\|^2 = \sum_{i=1}^{100} (\beta_0 + \beta_1 x_i)^2 - 2y_i(\beta_0 + \beta_1 x_i) + y_i^2$$

and we want to find β such that $C(\beta)$ is minimized.

The derivative of the cost/loss function

Computing $\partial C(\beta)/\partial \beta_0$ and $\partial C(\beta)/\partial \beta_1$ we can show that the gradient can be written as

$$\nabla_\beta C(\beta) = (\partial C(\beta)/\partial \beta_0, \partial C(\beta)/\partial \beta_1)^T = 2 \left[\begin{array}{c} \sum_{i=1}^{100} (\beta_0 + \beta_1 x_i - y_i) \\ \sum_{i=1}^{100} (x_i(\beta_0 + \beta_1 x_i) - y_i x_i) \end{array} \right] = 2X^T(X\beta - \mathbf{y}),$$

where X is the design matrix defined above.

The Hessian matrix

The Hessian matrix of $C(\beta)$ is given by

$$\hat{H} \equiv \begin{bmatrix} \frac{\partial^2 C(\beta)}{\partial \beta_0^2} & \text{amp;} \frac{\partial^2 C(\beta)}{\partial \beta_0 \partial \beta_1} \\ \frac{\partial^2 C(\beta)}{\partial \beta_0 \partial \beta_1} & \text{amp;} \frac{\partial^2 C(\beta)}{\partial \beta_1^2} & \text{amp;} \end{bmatrix} = 2X^T X.$$

This result implies that $C(\beta)$ is a convex function since the matrix $X^T X$ always is positive semi-definite.

Simple program

We can now write a program that minimizes $C(\beta)$ using the gradient descent method with a constant learning rate γ according to

$$\beta_{k+1} = \beta_k - \gamma \nabla_{\beta} C(\beta_k), \quad k = 0, 1, \dots$$

We can use the expression we computed for the gradient and let use a β_0 be chosen randomly and let $\gamma = 0.001$. Stop iterating when $\|\nabla_{\beta} C(\beta_k)\| \leq \epsilon = 10^{-8}$.

And finally we can compare our solution for β with the analytic result given by $\beta = (X^T X)^{-1} X^T \mathbf{y}$.

Gradient Descent Example

Here our simple example

And a corresponding example using scikit-learn

Gradient descent and Ridge

We have also discussed Ridge regression where the loss function contains a regularized term given by the L_2 norm of β ,

$$C_{\text{ridge}}(\beta) = \|X\beta - \mathbf{y}\|^2 + \lambda \|\beta\|^2, \quad \lambda \geq 0.$$

In order to minimize $C_{\text{ridge}}(\beta)$ using GD we only have adjust the gradient as follows

$$\nabla_{\beta} C_{\text{ridge}}(\beta) = 2 \left[\frac{\sum_{i=1}^{100} (\beta_0 + \beta_1 x_i - y_i)}{\sum_{i=1}^{100} (x_i (\beta_0 + \beta_1 x_i) - y_i x_i)} \right] + 2\lambda \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = 2(X^T(X\beta - \mathbf{y}) + \lambda\beta).$$

We can easily extend our program to minimize $C_{\text{ridge}}(\beta)$ using gradient descent and compare with the analytical solution given by

$$\beta_{\text{ridge}} = (X^T X + \lambda I_{2 \times 2})^{-1} X^T \mathbf{y}.$$

Program example for gradient descent with Ridge Regression

Using gradient descent methods, limitations

- **Gradient descent (GD) finds local minima of our function.** Since the GD algorithm is deterministic, if it converges, it will converge to a local minimum of our energy function. Because in ML we are often dealing with extremely rugged landscapes with many local minima, this can lead to poor performance.

- **GD is sensitive to initial conditions.** One consequence of the local nature of GD is that initial conditions matter. Depending on where one starts, one will end up at a different local minima. Therefore, it is very important to think about how one initializes the training process. This is true for GD as well as more complicated variants of GD.
- **Gradients are computationally expensive to calculate for large datasets.** In many cases in statistics and ML, the energy function is a sum of terms, with one term for each data point. For example, in linear regression, $E \propto \sum_{i=1}^n (y_i - \mathbf{w}^T \cdot \mathbf{x}_i)^2$; for logistic regression, the square error is replaced by the cross entropy. To calculate the gradient we have to sum over *all* n data points. Doing this at every GD step becomes extremely computationally expensive. An ingenious solution to this, is to calculate the gradients using small subsets of the data called “mini batches”. This has the added benefit of introducing stochasticity into our algorithm.
- **GD is very sensitive to choices of learning rates.** GD is extremely sensitive to the choice of learning rates. If the learning rate is very small, the training process take an extremely long time. For larger learning rates, GD can diverge and give poor results. Furthermore, depending on what the local landscape looks like, we have to modify the learning rates to ensure convergence. Ideally, we would *adaptively* choose the learning rates to match the landscape.
- **GD treats all directions in parameter space uniformly.** Another major drawback of GD is that unlike Newton’s method, the learning rate for GD is the same in all directions in parameter space. For this reason, the maximum learning rate is set by the behavior of the steepest direction and this can significantly slow down training. Ideally, we would like to take large steps in flat directions and small steps in steep directions. Since we are exploring rugged landscapes where curvatures change, this requires us to keep track of not only the gradient but second derivatives. The ideal scenario would be to calculate the Hessian but this proves to be too computationally expensive.
- GD can take exponential time to escape saddle points, even with random initialization. As we mentioned, GD is extremely sensitive to initial condition since it determines the particular local minimum GD would eventually reach. However, even with a good initialization scheme, through the introduction of randomness, GD can still take exponential time to escape saddle points.

Stochastic Gradient Descent

Stochastic gradient descent (SGD) and variants thereof address some of the shortcomings of the Gradient descent method discussed above.

The underlying idea of SGD comes from the observation that the cost function, which we want to minimize, can almost always be written as a sum over n data points $\{\mathbf{x}_i\}_{i=1}^n$,

$$C(\beta) = \sum_{i=1}^n c_i(\mathbf{x}_i, \beta).$$

Computation of gradients

This in turn means that the gradient can be computed as a sum over i -gradients

$$\nabla_{\beta} C(\beta) = \sum_i^n \nabla_{\beta} c_i(\mathbf{x}_i, \beta).$$

Stochasticity/randomness is introduced by only taking the gradient on a subset of the data called minibatches. If there are n data points and the size of each minibatch is M , there will be n/M minibatches. We denote these minibatches by B_k where $k = 1, \dots, n/M$.

SGD example

As an example, suppose we have 10 data points $(\mathbf{x}_1, \dots, \mathbf{x}_{10})$ and we choose to have $M = 5$ minibatches, then each minibatch contains two data points. In particular we have $B_1 = (\mathbf{x}_1, \mathbf{x}_2), \dots, B_5 = (\mathbf{x}_9, \mathbf{x}_{10})$. Note that if you choose $M = 1$ you have only a single batch with all data points and on the other extreme, you may choose $M = n$ resulting in a minibatch for each datapoint, i.e $B_k = \mathbf{x}_k$.

The idea is now to approximate the gradient by replacing the sum over all data points with a sum over the data points in one the minibatches picked at random in each gradient descent step

$$\nabla_{\beta} C(\beta) = \sum_{i=1}^n \nabla_{\beta} c_i(\mathbf{x}_i, \beta) \rightarrow \sum_{i \in B_k}^n \nabla_{\beta} c_i(\mathbf{x}_i, \beta).$$

The gradient step

Thus a gradient descent step now looks like

$$\beta_{j+1} = \beta_j - \gamma_j \sum_{i \in B_k}^n \nabla_{\beta} c_i(\mathbf{x}_i, \beta)$$

where k is picked at random with equal probability from $[1, n/M]$. An iteration over the number of minibatches (n/M) is commonly referred to as an epoch. Thus it is typical to choose a number of epochs and for each epoch iterate over the number of minibatches, as exemplified in the code below.

Simple example code

Taking the gradient only on a subset of the data has two important benefits. First, it introduces randomness which decreases the chance that our optimization scheme gets stuck in a local minima. Second, if the size of the minibatches are small relative to the number of datapoints ($M < n$), the computation of the gradient is much cheaper since we sum over the datapoints in the k -th minibatch and not all n datapoints.

When do we stop?

A natural question is when do we stop the search for a new minimum? One possibility is to compute the full gradient after a given number of epochs and check if the norm of the gradient is smaller than some threshold and stop if true. However, the condition that the gradient is zero is valid also for local minima, so this would only tell us that we are close to a local/global minimum. However, we could also evaluate the cost function at this point, store the result and continue the search. If the test kicks in at a later stage we can compare the values of the cost function and keep the β that gave the lowest value.

Slightly different approach

Another approach is to let the step length γ_j depend on the number of epochs in such a way that it becomes very small after a reasonable time such that we do not move at all.

As an example, let $e = 0, 1, 2, 3, \dots$ denote the current epoch and let $t_0, t_1 > 0$ be two fixed numbers. Furthermore, let $t = e \cdot m + i$ where m is the number of minibatches and $i = 0, \dots, m - 1$. Then the function

$$\gamma_j(t; t_0, t_1) = \frac{t_0}{t + t_1}$$

goes to zero as the number of epochs gets large. I.e. we start with a step length $\gamma_j(0; t_0, t_1) = t_0/t_1$ which decays in time t .

In this way we can fix the number of epochs, compute β and evaluate the cost function at the end. Repeating the computation will give a different result since the scheme is random by design. Then we pick the final β that gives the lowest value of the cost function.

Program for stochastic gradient

Challenge: try to write a similar code for a Logistic Regression case.

Momentum based GD

The stochastic gradient descent (SGD) is almost always used with a *momentum* or inertia term that serves as a memory of the direction we are moving in parameter space. This is typically implemented as follows

$$\begin{aligned}\mathbf{v}_t &= \gamma \mathbf{v}_{t-1} + \eta_t \nabla_{\theta} E(\boldsymbol{\theta}_t) \\ \boldsymbol{\theta}_{t+1} &= \boldsymbol{\theta}_t - \mathbf{v}_t,\end{aligned}\tag{2}$$

where we have introduced a momentum parameter γ , with $0 \leq \gamma \leq 1$, and for brevity we dropped the explicit notation to indicate the gradient is to be taken over a different mini-batch at each step. We call this algorithm gradient descent with momentum (GDM). From these equations, it is clear that \mathbf{v}_t is a running average of recently encountered gradients and $(1 - \gamma)^{-1}$ sets the characteristic time scale for the memory used in the averaging procedure. Consistent with this, when $\gamma = 0$, this just reduces down to ordinary SGD as discussed earlier. An equivalent way of writing the updates is

$$\Delta \boldsymbol{\theta}_{t+1} = \gamma \Delta \boldsymbol{\theta}_t - \eta_t \nabla_{\theta} E(\boldsymbol{\theta}_t),$$

where we have defined $\Delta \boldsymbol{\theta}_t = \boldsymbol{\theta}_t - \boldsymbol{\theta}_{t-1}$.

More on momentum based approaches

Let us try to get more intuition from these equations. It is helpful to consider a simple physical analogy with a particle of mass m moving in a viscous medium with drag coefficient μ and potential $E(\mathbf{w})$. If we denote the particle's position by \mathbf{w} , then its motion is described by

$$m \frac{d^2 \mathbf{w}}{dt^2} + \mu \frac{d\mathbf{w}}{dt} = -\nabla_{\mathbf{w}} E(\mathbf{w}).$$

We can discretize this equation in the usual way to get

$$m \frac{\mathbf{w}_{t+\Delta t} - 2\mathbf{w}_t + \mathbf{w}_{t-\Delta t}}{(\Delta t)^2} + \mu \frac{\mathbf{w}_{t+\Delta t} - \mathbf{w}_t}{\Delta t} = -\nabla_{\mathbf{w}} E(\mathbf{w}).$$

Rearranging this equation, we can rewrite this as

$$\Delta \mathbf{w}_{t+\Delta t} = -\frac{(\Delta t)^2}{m + \mu \Delta t} \nabla_{\mathbf{w}} E(\mathbf{w}) + \frac{m}{m + \mu \Delta t} \Delta \mathbf{w}_t.$$

Momentum parameter

Notice that this equation is identical to previous one if we identify the position of the particle, \mathbf{w} , with the parameters $\boldsymbol{\theta}$. This allows us to identify the momentum parameter and learning rate with the mass of the particle and the viscous drag as:

$$\gamma = \frac{m}{m + \mu \Delta t}, \quad \eta = \frac{(\Delta t)^2}{m + \mu \Delta t}.$$

Thus, as the name suggests, the momentum parameter is proportional to the mass of the particle and effectively provides inertia. Furthermore, in the

large viscosity/small learning rate limit, our memory time scales as $(1 - \gamma)^{-1} \approx m/(\mu\Delta t)$.

Why is momentum useful? SGD momentum helps the gradient descent algorithm gain speed in directions with persistent but small gradients even in the presence of stochasticity, while suppressing oscillations in high-curvature directions. This becomes especially important in situations where the landscape is shallow and flat in some directions and narrow and steep in others. It has been argued that first-order methods (with appropriate initial conditions) can perform comparable to more expensive second order methods, especially in the context of complex deep learning models.

These beneficial properties of momentum can sometimes become even more pronounced by using a slight modification of the classical momentum algorithm called Nesterov Accelerated Gradient (NAG).

In the NAG algorithm, rather than calculating the gradient at the current parameters, $\nabla_{\theta} E(\theta_t)$, one calculates the gradient at the expected value of the parameters given our current momentum, $\nabla_{\theta} E(\theta_t + \gamma \mathbf{v}_{t-1})$. This yields the NAG update rule

$$\begin{aligned}\mathbf{v}_t &= \gamma \mathbf{v}_{t-1} + \eta_t \nabla_{\theta} E(\theta_t + \gamma \mathbf{v}_{t-1}) \\ \theta_{t+1} &= \theta_t - \mathbf{v}_t.\end{aligned}\tag{3}$$

One of the major advantages of NAG is that it allows for the use of a larger learning rate than GDM for the same choice of γ .

Second moment of the gradient

In stochastic gradient descent, with and without momentum, we still have to specify a schedule for tuning the learning rates η_t as a function of time. As discussed in the context of Newton’s method, this presents a number of dilemmas. The learning rate is limited by the steepest direction which can change depending on the current position in the landscape. To circumvent this problem, ideally our algorithm would keep track of curvature and take large steps in shallow, flat directions and small steps in steep, narrow directions. Second-order methods accomplish this by calculating or approximating the Hessian and normalizing the learning rate by the curvature. However, this is very computationally expensive for extremely large models. Ideally, we would like to be able to adaptively change the step size to match the landscape without paying the steep computational price of calculating or approximating Hessians.

Recently, a number of methods have been introduced that accomplish this by tracking not only the gradient, but also the second moment of the gradient. These methods include AdaGrad, AdaDelta, RMS-Prop, and ADAM.

RMS prop

In RMS prop, in addition to keeping a running average of the first moment of the gradient, we also keep track of the second moment denoted by $\mathbf{s}_t = \mathbb{E}[\mathbf{g}_t^2]$. The update rule for RMS prop is given by

$$\begin{aligned}\mathbf{g}_t &= \nabla_{\theta} E(\boldsymbol{\theta}) \\ \mathbf{s}_t &= \beta \mathbf{s}_{t-1} + (1 - \beta) \mathbf{g}_t^2 \\ \boldsymbol{\theta}_{t+1} &= \boldsymbol{\theta}_t - \eta_t \frac{\mathbf{g}_t}{\sqrt{\mathbf{s}_t + \epsilon}},\end{aligned}\tag{4}$$

where β controls the averaging time of the second moment and is typically taken to be about $\beta = 0.9$, η_t is a learning rate typically chosen to be 10^{-3} , and $\epsilon \sim 10^{-8}$ is a small regularization constant to prevent divergences. Multiplication and division by vectors is understood as an element-wise operation. It is clear from this formula that the learning rate is reduced in directions where the norm of the gradient is consistently large. This greatly speeds up the convergence by allowing us to use a larger learning rate for flat directions.

ADAM optimizer

A related algorithm is the ADAM optimizer. In ADAM, we keep a running average of both the first and second moment of the gradient and use this information to adaptively change the learning rate for different parameters. In addition to keeping a running average of the first and second moments of the gradient (i.e. $\mathbf{m}_t = \mathbb{E}[\mathbf{g}_t]$ and $\mathbf{s}_t = \mathbb{E}[\mathbf{g}_t^2]$, respectively), ADAM performs an additional bias correction to account for the fact that we are estimating the first two moments of the gradient using a running average (denoted by the hats in the update rule below). The update rule for ADAM is given by (where multiplication and division are once again understood to be element-wise operations below)

$$\begin{aligned}\mathbf{g}_t &= \nabla_{\theta} E(\boldsymbol{\theta}) \\ \mathbf{m}_t &= \beta_1 \mathbf{m}_{t-1} + (1 - \beta_1) \mathbf{g}_t \\ \mathbf{s}_t &= \beta_2 \mathbf{s}_{t-1} + (1 - \beta_2) \mathbf{g}_t^2 \\ \hat{\mathbf{m}}_t &= \frac{\mathbf{m}_t}{1 - \beta_1^t} \\ \hat{\mathbf{s}}_t &= \frac{\mathbf{s}_t}{1 - \beta_2^t} \\ \boldsymbol{\theta}_{t+1} &= \boldsymbol{\theta}_t - \eta_t \frac{\hat{\mathbf{m}}_t}{\sqrt{\hat{\mathbf{s}}_t + \epsilon}},\end{aligned}\tag{5}$$

where β_1 and β_2 set the memory lifetime of the first and second moment and are typically taken to be 0.9 and 0.99 respectively, and η and ϵ are identical to RMSprop.

Like in RMSprop, the effective step size of a parameter depends on the magnitude of its gradient squared. To understand this better, let us rewrite this expression in terms of the variance $\sigma_t^2 = \hat{\mathbf{s}}_t - (\hat{\mathbf{m}}_t)^2$. Consider a single parameter θ_t . The update rule for this parameter is given by

$$\Delta\theta_{t+1} = -\eta_t \frac{\hat{m}_t}{\sqrt{\sigma_t^2 + m_t^2 + \epsilon}}.$$

Practical tips

- **Randomize the data when making mini-batches.** It is always important to randomly shuffle the data when forming mini-batches. Otherwise, the gradient descent method can fit spurious correlations resulting from the order in which data is presented.
- **Transform your inputs.** Learning becomes difficult when our landscape has a mixture of steep and flat directions. One simple trick for minimizing these situations is to standardize the data by subtracting the mean and normalizing the variance of input variables. Whenever possible, also decorrelate the inputs. To understand why this is helpful, consider the case of linear regression. It is easy to show that for the squared error cost function, the Hessian of the energy matrix is just the correlation matrix between the inputs. Thus, by standardizing the inputs, we are ensuring that the landscape looks homogeneous in all directions in parameter space. Since most deep networks can be viewed as linear transformations followed by a non-linearity at each layer, we expect this intuition to hold beyond the linear case.
- **Monitor the out-of-sample performance.** Always monitor the performance of your model on a validation set (a small portion of the training data that is held out of the training process to serve as a proxy for the test set. If the validation error starts increasing, then the model is beginning to overfit. Terminate the learning process. This *early stopping* significantly improves performance in many settings.
- **Adaptive optimization methods don't always have good generalization.** Recent studies have shown that adaptive methods such as ADAM, RMSProp, and AdaGrad tend to have poor generalization compared to SGD or SGD with momentum, particularly in the high-dimensional limit (i.e. the number of parameters exceeds the number of data points). Although it is not clear at this stage why these methods perform so well in training deep neural networks, simpler procedures like properly-tuned SGD may work as well or better in these applications.

Geron's text, see chapter 11, has several interesting discussions.

Automatic differentiation

Automatic differentiation (AD), also called algorithmic differentiation or computational differentiation, is a set of techniques to numerically evaluate the derivative of a function specified by a computer program. AD exploits the fact that every computer program, no matter how complicated, executes a sequence of elementary arithmetic operations (addition, subtraction, multiplication, division, etc.) and elementary functions (exp, log, sin, cos, etc.). By applying the chain rule repeatedly to these operations, derivatives of arbitrary order can be computed automatically, accurately to working precision, and using at most a small constant factor more arithmetic operations than the original program.

Automatic differentiation is neither:

- Symbolic differentiation, nor
- Numerical differentiation (the method of finite differences).

Symbolic differentiation can lead to inefficient code and faces the difficulty of converting a computer program into a single expression, while numerical differentiation can introduce round-off errors in the discretization process and cancellation.

Python has tools for so-called **automatic differentiation**. Consider the following example

$$f(x) = \sin(2\pi x + x^2)$$

which has the following derivative

$$f'(x) = \cos(2\pi x + x^2) (2\pi + 2x)$$

Using **autograd** we have

Using autograd

Here we experiment with what kind of functions Autograd is capable of finding the gradient of. The following Python functions are just meant to illustrate what Autograd can do, but please feel free to experiment with other, possibly more complicated, functions as well.

Autograd with more complicated functions

To differentiate with respect to two (or more) arguments of a Python function, Autograd needs to know at which variable the function is being differentiated with respect to.

Note that the grad function will not produce the true gradient of the function. The true gradient of a function with two or more variables will produce a vector, where each element is the function differentiated w.r.t a variable.

More complicated functions using the elements of their arguments directly

Note that in this case, when sending an array as input argument, the output from Autograd is another array. This is the true gradient of the function, as opposed to the function in the previous example. By using arrays to represent the variables, the output from Autograd might be easier to work with, as the output is closer to what one could expect from a gradient-evaluating function.

Functions using mathematical functions from Numpy

More autograd

And with loops

Using recursion

Note that if n is equal to zero or one, Autograd will give an error message. This message appears when the output is independent on input.

Unsupported functions

Autograd supports many features. However, there are some functions that is not supported (yet) by Autograd.

Assigning a value to the variable being differentiated with respect to Here, Autograd tells us that an 'ArrayBox' does not support item assignment. The item assignment is done when the program tries to assign $x[2]$ to the value 3. However, Autograd has implemented the computation of the derivative such that this assignment is not possible.

The syntax `a.dot(b)` when finding the dot product

Here we are told that the 'dot' function does not belong to Autograd's version of a Numpy array. To overcome this, an alternative syntax which also computed the dot product can be used:

Recommended to avoid

The documentation recommends to avoid inplace operations such as

Standard steepest descent

Before we proceed, we would like to discuss the approach called the **standard Steepest descent**, which again leads to us having to be able to compute a matrix. It belongs to the class of Conjugate Gradient methods (CG).

[The success of the CG method](#) for finding solutions of non-linear problems is based on the theory of conjugate gradients for linear systems of equations. It

belongs to the class of iterative methods for solving problems from linear algebra of the type

$$\hat{A}\hat{x} = \hat{b}.$$

In the iterative process we end up with a problem like

$$\hat{r} = \hat{b} - \hat{A}\hat{x},$$

where \hat{r} is the so-called residual or error in the iterative process.

When we have found the exact solution, $\hat{r} = 0$.

Gradient method

The residual is zero when we reach the minimum of the quadratic equation

$$P(\hat{x}) = \frac{1}{2}\hat{x}^T \hat{A}\hat{x} - \hat{x}^T \hat{b},$$

with the constraint that the matrix \hat{A} is positive definite and symmetric. This defines also the Hessian and we want it to be positive definite.

Steepest descent method

We denote the initial guess for \hat{x} as \hat{x}_0 . We can assume without loss of generality that

$$\hat{x}_0 = 0,$$

or consider the system

$$\hat{A}\hat{z} = \hat{b} - \hat{A}\hat{x}_0,$$

instead.

Steepest descent method

One can show that the solution \hat{x} is also the unique minimizer of the quadratic form

$$f(\hat{x}) = \frac{1}{2}\hat{x}^T \hat{A}\hat{x} - \hat{x}^T \hat{b}, \quad \hat{x} \in \mathbf{R}^n.$$

This suggests taking the first basis vector \hat{r}_1 (see below for definition) to be the gradient of f at $\hat{x} = \hat{x}_0$, which equals

$$\hat{A}\hat{x}_0 - \hat{b},$$

and $\hat{x}_0 = 0$ it is equal $-\hat{b}$.

Final expressions

We can compute the residual iteratively as

$$\hat{r}_{k+1} = \hat{b} - \hat{A}\hat{x}_{k+1},$$

which equals

$$\hat{b} - \hat{A}(\hat{x}_k + \alpha_k \hat{r}_k),$$

or

$$(\hat{b} - \hat{A}\hat{x}_k) - \alpha_k \hat{A}\hat{r}_k,$$

which gives

$$\alpha_k = \frac{\hat{r}_k^T \hat{r}_k}{\hat{r}_k^T \hat{A}\hat{r}_k}$$

leading to the iterative scheme

$$\hat{x}_{k+1} = \hat{x}_k - \alpha_k \hat{r}_k,$$

Code examples for steepest descent

Simple codes for steepest descent and conjugate gradient using a 2×2 matrix, in c++, Python code to come

The routine for the steepest descent method

Steepest descent example

And then as contour plot Find guesses Run it! What happened?

Conjugate gradient method

In the CG method we define so-called conjugate directions and two vectors \hat{s} and \hat{t} are said to be conjugate if

$$\hat{s}^T \hat{A}\hat{t} = 0.$$

The philosophy of the CG method is to perform searches in various conjugate directions of our vectors \hat{x}_i obeying the above criterion, namely

$$\hat{x}_i^T \hat{A}\hat{x}_j = 0.$$

Two vectors are conjugate if they are orthogonal with respect to this inner product. Being conjugate is a symmetric relation: if \hat{s} is conjugate to \hat{t} , then \hat{t} is conjugate to \hat{s} .

Conjugate gradient method

An example is given by the eigenvectors of the matrix

$$\hat{v}_i^T \hat{A} \hat{v}_j = \lambda \hat{v}_i^T \hat{v}_j,$$

which is zero unless $i = j$.

Conjugate gradient method

Assume now that we have a symmetric positive-definite matrix \hat{A} of size $n \times n$. At each iteration $i + 1$ we obtain the conjugate direction of a vector

$$\hat{x}_{i+1} = \hat{x}_i + \alpha_i \hat{p}_i.$$

We assume that \hat{p}_i is a sequence of n mutually conjugate directions. Then the \hat{p}_i form a basis of R^n and we can expand the solution $\hat{A}\hat{x} = \hat{b}$ in this basis, namely

$$\hat{x} = \sum_{i=1}^n \alpha_i \hat{p}_i.$$

Conjugate gradient method

The coefficients are given by

$$\mathbf{A}\mathbf{x} = \sum_{i=1}^n \alpha_i \mathbf{A}\mathbf{p}_i = \mathbf{b}.$$

Multiplying with \hat{p}_k^T from the left gives

$$\hat{p}_k^T \hat{A} \hat{x} = \sum_{i=1}^n \alpha_i \hat{p}_k^T \hat{A} \hat{p}_i = \hat{p}_k^T \hat{b},$$

and we can define the coefficients α_k as

$$\alpha_k = \frac{\hat{p}_k^T \hat{b}}{\hat{p}_k^T \hat{A} \hat{p}_k}$$

Conjugate gradient method and iterations

If we choose the conjugate vectors \hat{p}_k carefully, then we may not need all of them to obtain a good approximation to the solution \hat{x} . We want to regard the conjugate gradient method as an iterative method. This will us to solve systems where n is so large that the direct method would take too much time.

We denote the initial guess for \hat{x} as \hat{x}_0 . We can assume without loss of generality that

$$\hat{x}_0 = 0,$$

or consider the system

$$\hat{A}\hat{z} = \hat{b} - \hat{A}\hat{x}_0,$$

instead.

Conjugate gradient method

One can show that the solution \hat{x} is also the unique minimizer of the quadratic form

$$f(\hat{x}) = \frac{1}{2} \hat{x}^T \hat{A} \hat{x} - \hat{x}^T \hat{b}, \quad \hat{x} \in \mathbf{R}^n.$$

This suggests taking the first basis vector \hat{p}_1 to be the gradient of f at $\hat{x} = \hat{x}_0$, which equals

$$\hat{A} \hat{x}_0 - \hat{b},$$

and $\hat{x}_0 = 0$ it is equal $-\hat{b}$. The other vectors in the basis will be conjugate to the gradient, hence the name conjugate gradient method.

Conjugate gradient method

Let \hat{r}_k be the residual at the k -th step:

$$\hat{r}_k = \hat{b} - \hat{A} \hat{x}_k.$$

Note that \hat{r}_k is the negative gradient of f at $\hat{x} = \hat{x}_k$, so the gradient descent method would be to move in the direction \hat{r}_k . Here, we insist that the directions \hat{p}_k are conjugate to each other, so we take the direction closest to the gradient \hat{r}_k under the conjugacy constraint. This gives the following expression

$$\hat{p}_{k+1} = \hat{r}_k - \frac{\hat{p}_k^T \hat{A} \hat{r}_k}{\hat{p}_k^T \hat{A} \hat{p}_k} \hat{p}_k.$$

Conjugate gradient method

We can also compute the residual iteratively as

$$\hat{r}_{k+1} = \hat{b} - \hat{A} \hat{x}_{k+1},$$

which equals

$$\hat{b} - \hat{A}(\hat{x}_k + \alpha_k \hat{p}_k),$$

or

$$(\hat{b} - \hat{A} \hat{x}_k) - \alpha_k \hat{A} \hat{p}_k,$$

which gives

$$\hat{r}_{k+1} = \hat{r}_k - \hat{A} \hat{p}_k,$$

Simple implementation of the Conjugate gradient algorithm

Broyden–Fletcher–Goldfarb–Shanno algorithm

The optimization problem is to minimize $f(\mathbf{x})$ where \mathbf{x} is a vector in R^n , and f is a differentiable scalar function. There are no constraints on the values that \mathbf{x} can take.

The algorithm begins at an initial estimate for the optimal value \mathbf{x}_0 and proceeds iteratively to get a better estimate at each stage.

The search direction p_k at stage k is given by the solution of the analogue of the Newton equation

$$B_k \mathbf{p}_k = -\nabla f(\mathbf{x}_k),$$

where B_k is an approximation to the Hessian matrix, which is updated iteratively at each stage, and $\nabla f(\mathbf{x}_k)$ is the gradient of the function evaluated at x_k . A line search in the direction p_k is then used to find the next point x_{k+1} by minimising

$$f(\mathbf{x}_k + \alpha \mathbf{p}_k),$$

over the scalar $\alpha > 0$.