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# Gradient descent

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For the analytical method called "steepest descent", see Method of steepest descent.

Gradient descent is a first-order iterative optimization algorithm for finding a local minimum of a differentiable function. To find a local minimum of a function using gradient descent, we take steps proportional to the negative of the gradient (or approximate gradient) of the function at the current point. But if we instead take steps proportional to the positive of the gradient, we approach a local maximum of that function; the procedure is then known as gradient ascent. Gradient descent is generally attributed to Cauchy, who first suggested it in 1847,[1] but its convergence properties for non-linear optimization problems were first studied by Haskell Curry in 1944.[2]

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# Description [edit]

Gradient descent is based on the observation that if the multi-variable function  $F(\mathbf{x})$  is defined and differentiable in a neighborhood of a point  ${f a}$ , then  $F({f x})$  decreases fastest if one goes from  ${f a}$ in the direction of the negative gradient of F at  $\mathbf{a}, -\nabla F(\mathbf{a})$ . It follows that, if

$$\mathbf{a}_{n+1} = \mathbf{a}_n - \gamma 
abla F(\mathbf{a}_n)$$

for  $\gamma \in \mathbb{R}_+$  small enough, then  $F(\mathbf{a_n}) \geq F(\mathbf{a_{n+1}})$ . In other words, the term  $\gamma \nabla F(\mathbf{a})$  is subtracted from a because we want to move against the gradient, toward the local minimum. With this observation in mind, one starts with a guess  $\mathbf{x_0}$  for a local minimum of F, and considers the sequence  $\mathbf{x}_0, \mathbf{x}_1, \mathbf{x}_2, \dots$  such that

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \gamma_n \nabla F(\mathbf{x}_n), \ n \geq 0.$$

We have a monotonic sequence

$$F(\mathbf{x}_0) \geq F(\mathbf{x}_1) \geq F(\mathbf{x}_2) \geq \cdots,$$

so hopefully the sequence  $(\mathbf{x}_n)$  converges to the desired local minimum. Note that the value of the *step size*  $m{\gamma}$  is allowed to change at every iteration. With certain assumptions on the function  $m{F}$ (for example, F convex and  $\nabla F$  Lipschitz) and particular choices of  $\gamma$  (e.g., chosen either via a line search that satisfies the Wolfe conditions, or the Barzilai–Borwein method<sup>[3][4]</sup> shown as

$$\gamma_n = \frac{\left| \left(\mathbf{x}_n - \mathbf{x}_{n-1}\right)^T \left[ \nabla F(\mathbf{x}_n) - \nabla F(\mathbf{x}_{n-1}) \right] \right|}{\left\| \nabla F(\mathbf{x}_n) - \nabla F(\mathbf{x}_{n-1}) \right\|^2}$$

convergence to a local minimum can be guaranteed. When the function F is convex, all local minima are also global minima, so in this case gradient descent can converge to the global solution.

This process is illustrated in the adjacent picture. Here  ${m F}$  is assumed to be defined on the plane, and that its graph has a bowl shape. The blue curves are the contour lines, that is, the regions on which the value of F is constant. A red arrow originating at a point shows the direction of the negative gradient at that point. Note that the (negative) gradient at a point is orthogonal to the contour line going through that point. We see that gradient descent leads us to the bottom of the bowl, that is, to the point where the value of the function  $m{F}$  is minimal.

## An analogy for understanding gradient descent [edit]

The basic intuition behind gradient descent can be illustrated by a hypothetical scenario. A person is stuck in the mountains and is trying to get down (i.e. trying to find the global minimum). There is heavy fog such that visibility is extremely low. Therefore, the path down the mountain is not visible, so they must use local information to find the minimum. They can use the method of gradient descent, which involves looking at the steepness of the hill at their current position, then proceeding in the direction with the steepest descent (i.e. downhill). If they were trying to find the top of the mountain (i.e. the maximum), then they would proceed in the direction of steepest ascent (i.e. uphill). Using this method, they would eventually find their way down the mountain or possibly get stuck in some hole (i.e. local minimum or saddle point), like a mountain lake. However, assume also that the steepness of the hill is not immediately



Illustration of gradient descent on a series of level sets

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obvious with simple observation, but rather it requires a sophisticated instrument to measure, which the person

happens to have at the moment. It takes quite some time to measure the steepness of the hill with the instrument, thus they should minimize their use of the instrument if they wanted to get down the mountain before sunset. The difficulty then is choosing the frequency at which they should measure the steepness of the hill so not to go off track.

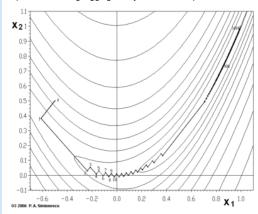
In this analogy, the person represents the algorithm, and the path taken down the mountain represents the sequence of parameter settings that the algorithm will explore. The steepness of the hill represents the slope of the error surface at that point. The instrument used to measure steepness is differentiation (the slope of the error surface can be calculated by taking the derivative of the squared error function at that point). The direction they choose to travel in aligns with the gradient of the error surface at that point. The amount of time they travel before taking another measurement is the learning rate of the algorithm. See Backpropagation § Limitations for a discussion of the limitations of this type of "hill descending" algorithm.

## Examples [edit]

Gradient descent has problems with pathological functions such as the Rosenbrock function shown here.

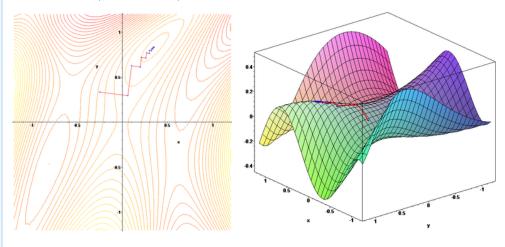
$$f(x_1, x_2) = (1 - x_1)^2 + 100(x_2 - x_1^2)^2.$$

The Rosenbrock function has a narrow curved valley which contains the minimum. The bottom of the valley is very flat. Because of the curved flat valley the optimization is zigzagging slowly with small step sizes towards the minimum.



The zigzagging nature of the method is also evident below, where the gradient descent method is applied to

$$F(x,y) = \sin\left(\frac{1}{2}x^2 - \frac{1}{4}y^2 + 3\right)\cos(2x + 1 - e^y).$$



# Solution of a linear system [edit]

Gradient descent can be used to solve a system of linear equations, reformulated as a quadratic minimization problem, e.g., using linear least squares. The solution of

$$A\mathbf{x} - \mathbf{b} = 0$$

in the sense of linear least squares is defined as minimizing the function

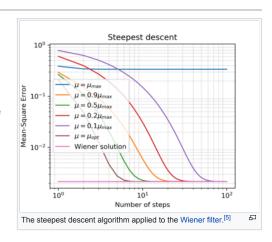
$$F(\mathbf{x}) = \|A\mathbf{x} - \mathbf{b}\|^2.$$

In traditional linear least squares for real  ${m A}$  and  ${m b}$  the Euclidean norm is used, in which case

$$\nabla F(\mathbf{x}) = 2A^T(A\mathbf{x} - \mathbf{b}).$$

In this case, the line search minimization, finding the locally optimal step size  $\gamma$  on every iteration, can be performed analytically, and explicit formulas for the locally optimal  $\gamma$  are known. [6]

The algorithm is rarely used for solving linear equations, with the conjugate gradient method being one of the most popular alternatives. The number of gradient descent iterations is commonly proportional to the spectral condition number  $\kappa(A)$  of the system matrix A (the



ratio of the maximum to minimum eigenvalues of  $A^TA$ ), while the convergence of conjugate gradient method is typically determined by a square root of the condition number, i.e., is much faster. Both methods can benefit from preconditioning, where gradient descent may require less assumptions on the preconditioner.<sup>[7]</sup>

# Solution of a non-linear system [edit]

Gradient descent can also be used to solve a system of nonlinear equations. Below is an example that shows how to use the gradient descent to solve for three unknown variables,  $x_1$ ,  $x_2$ , and  $x_3$ . This example shows one iteration of the gradient descent.

Consider the nonlinear system of equations

$$\begin{cases} 3x_1 - \cos(x_2x_3) - \frac{3}{2} = 0 \\ 4x_1^2 - 625x_2^2 + 2x_2 - 1 = 0 \\ \exp(-x_1x_2) + 20x_3 + \frac{10\pi - 3}{3} = 0 \end{cases}$$

Let us introduce the associated function

$$G(\mathbf{x}) = egin{bmatrix} 3x_1 - \cos(x_2x_3) - rac{3}{2} \ 4x_1^2 - 625x_2^2 + 2x_2 - 1 \ \exp(-x_1x_2) + 20x_3 + rac{10\pi - 3}{3} \end{bmatrix},$$

where

$$\mathbf{x} = egin{bmatrix} x_1 \ x_2 \ x_3 \end{bmatrix}$$

One might now define the objective function

$$F(\mathbf{x}) = \frac{1}{2}G^{\mathrm{T}}(\mathbf{x})G(\mathbf{x}) = \frac{1}{2}\left[\left(3x_1 - \cos(x_2x_3) - \frac{3}{2}\right)^2 + \left(4x_1^2 - 625x_2^2 + 2x_2 - 1\right)^2 + \left(\exp(-x_1x_2) + 20x_3 + \frac{10\pi - 3}{3}\right)^2\right],$$

which we will attempt to minimize. As an initial guess, let us use

$$\mathbf{x}^{(0)} = \mathbf{0} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

We know that

$$\mathbf{x}^{(1)} = \mathbf{0} - \gamma_0 \nabla F(\mathbf{0}) = \mathbf{0} - \gamma_0 J_G(\mathbf{0})^{\mathrm{T}} G(\mathbf{0}),$$

where the Jacobian matrix  $oldsymbol{J_G}$  is given by

$$J_G(\mathtt{x}) = egin{bmatrix} 3 & \sin(x_2x_3)x_3 & \sin(x_2x_3)x_2 \ 8x_1 & -1250x_2 + 2 & 0 \ -x_2\exp\left(-x_1x_2
ight) & -x_1\exp(-x_1x_2) & 20 \end{bmatrix}.$$

We calculate

$$J_G(\mathbf{0}) = egin{bmatrix} 3 & 0 & 0 \ 0 & 2 & 0 \ 0 & 0 & 20 \end{bmatrix}, \qquad G(\mathbf{0}) = egin{bmatrix} -2.5 \ -1 \ 10.472 \end{bmatrix}.$$

Thus

$$\mathbf{x}^{(1)} = \mathbf{0} - \gamma_0 \begin{bmatrix} -7.5 \\ -2 \\ 209.44 \end{bmatrix},$$

and

$$F(0) = 0.5((-2.5)^2 + (-1)^2 + (10.472)^2) = 58.456.$$

Now, a suitable  $\gamma_0$  must be found such that

$$F\left(\mathbf{x}^{(1)}\right) \leq F\left(\mathbf{x}^{(0)}\right) = F(\mathbf{0}).$$

This can be done with any of a variety of line search algorithms. One might also simply guess  $\gamma_0=0.001$ , which gives

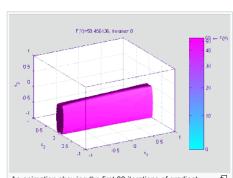
$$\mathbf{x}^{(1)} = \begin{bmatrix} 0.0075 \\ 0.002 \\ -0.20944 \end{bmatrix}.$$

Evaluating the objective function at this value, yields

$$F\left(\mathbf{x}^{(1)}\right) = 0.5\left((-2.48)^2 + (-1.00)^2 + (6.28)^2\right) = 23.306.$$

The decrease from  $F(\mathbf{0}) = 58.456$  to the next step's value of

$$F\left(\mathbf{x}^{(1)}\right) = 23.306$$



An animation showing the first 83 iterations of gradient descent applied to this example. Surfaces are isosurfaces of  $F(\mathbf{x}^{(n)})$  at current guess  $\mathbf{x}^{(n)}$ , and arrows show the direction of descent. Due to a small and constant step size, the convergence is slow.

is a sizable decrease in the objective function. Further steps would reduce its value further, until an approximate solution to the system was found.

## Comments [edit]

Gradient descent works in spaces of any number of dimensions, even in infinite-dimensional ones. In the latter case, the search space is typically a function space, and one calculates the Fréchet derivative of the functional to be minimized to determine the descent direction.<sup>[8]</sup>

That gradient descent works in any number of dimensions (finite number at least) can be seen as a consequence of the Cauchy-Schwarz inequality. That article proves that the magnitude of the inner (dot) product of two vectors of any dimension is maximized when the are colinear. In the case of gradient descent, that would be when the vector of independent variable adjustments is proportional to the gradient vector of partial derivatives.

The gradient descent can take many iterations to compute a local minimum with a required accuracy, if the curvature in different directions is very different for the given function. For such functions, preconditioning, which changes the geometry of the space to shape the function level sets like concentric circles, cures the slow convergence. Constructing and applying preconditioning can be computationally expensive, however.

The gradient descent can be combined with a line search, finding the locally optimal step size  $\gamma$  on every iteration. Performing the line search can be time-consuming. Conversely, using a fixed small  $\gamma$  can yield poor convergence.

Methods based on Newton's method and inversion of the Hessian using conjugate gradient techniques can be better alternatives. <sup>[9][10]</sup> Generally, such methods converge in fewer iterations, but the cost of each iteration is higher. An example is the BFGS method which consists in calculating on every step a matrix by which the gradient vector is multiplied to go into a "better" direction, combined with a more sophisticated line search algorithm, to find the "best" value of γ. For extremely large problems, where the computer-memory issues dominate, a limited-memory method such as L-BFGS should be used instead of BFGS or the steepest descent.

Gradient descent can be viewed as applying Euler's method for solving ordinary differential equations  $x'(t) = -\nabla f(x(t))$  to a gradient flow. In turn, this equation may be derived as an optimal controller<sup>[11]</sup> for the control system x'(t) = u(t) with u(t) given in feedback form  $u(t) = -\nabla f(x(t))$ .

#### Extensions [edit]

Gradient descent can be extended to handle constraints by including a projection onto the set of constraints. This method is only feasible when the projection is efficiently computable on a computer. Under suitable assumptions, this method converges. This method is a specific case of the forward-backward algorithm for monotone inclusions (which includes convex programming and variational inequalities).<sup>[12]</sup>

## Fast gradient methods [edit]

Another extension of gradient descent is due to Yurii Nesterov from 1983, [13] and has been subsequently generalized. He provides a simple modification of the algorithm that enables faster convergence for convex problems. For unconstrained smooth problems the method is called the Fast Gradient Method (FGM) or the Accelerated Gradient Method (AGM). Specifically, if the differentiable function F is convex and  $\nabla F$  is Lipschitz, and it is not assumed that F is strongly convex, then the error in the objective value generated at each step F by the gradient descent method will be bounded by  $O\left(\frac{1}{k}\right)$ . Using the Nesterov

acceleration technique, the error decreases at  $\mathcal{O}\left(\frac{1}{k^2}\right)$ . [14] It is known that the rate  $\mathcal{O}\left(k^{-2}\right)$  for the decrease of the cost function is optimal for first-order optimization methods. Nevertheless, there is the opportunity to improve the algorithm by reducing the constant factor. The optimized gradient method (OGM)[15] reduces that constant by a factor of two and is an optimal first-order method for large-scale problems.[16]

For constrained or non-smooth problems, Nesterov's FGM is called the fast proximal gradient method (FPGM), an acceleration of the proximal gradient method.

## The momentum method [edit]

Main article: Stochastic gradient descent § Momentum

Yet another extension, that reduces the risk of getting stuck in a local minimum, as well as speeds up the convergence considerably in cases where the process would otherwise zig-zag heavily, is the *momentum method*, which uses a momentum term in analogy to "the mass of Newtonian particles that move through a viscous medium in a conservative force field".<sup>[17]</sup> This method is often used as an extension to the backpropagation algorithms used to train artificial neural networks.<sup>[18][19]</sup>

# See also [edit]

- Conjugate gradient method
- Stochastic gradient descent
- Rprop
- Delta rule

- Wolfe conditions
- Preconditioning
- Broyden–Fletcher–Goldfarb–Shanno algorithm
- Davidon-Fletcher-Powell formula
- Nelder-Mead method
- Gauss-Newton algorithm
- Hill climbing
- Quantum annealing

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# Further reading [edit]

• Boyd, Stephen; Vandenberghe, Lieven (2004). "Unconstrained Minimization" (PDF). Convex Optimization. New York: Cambridge University Press. pp. 457–520. ISBN 0-521-83378-7.

## External links [edit]

- Using gradient descent in C++, Boost, Ublas for linear regression
   □
- Series of Khan Academy videos discusses gradient ascent
- Online book teaching gradient descent in deep neural network context 

   ☑
- "Gradient Descent, How Neural Networks Learn" & . 3Blue1Brown. October 16, 2017 via YouTube.

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