ECEN 434: Optimization for ECEN

Lecture 10: Descent Methods for Unconstrained Problems

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Unconstrained minimization problems

- Consider the unconstrained optimization problem:

$$\text{minimize}_{\boldsymbol{x} \in \mathbb{X}} \quad f(\boldsymbol{x})$$

where f is convex and twice continuously differentiable and $\mathbb{X}$ is a nonempty, open set

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  where f is convex and twice continuously differentiable and $\mathbb{X}$ is a nonempty, open set

- We will assume that the the minimum value of f is attainable, i.e., there exists an optimal point $\boldsymbol{x}^*$

- Since f is convex and differentiable, a necessary and sufficient condition for a point $\boldsymbol{x}^*$ to be optimal is

$$\nabla f(\boldsymbol{x}^*) = \mathbf{0}$$

  Thus, solving the unconstrained minimization problem is the same as finding a solution to the above system of equations

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- By this we mean an algorithm that computes a sequence of points $\boldsymbol{x}^{(0)}, \boldsymbol{x}^{(1)}, \ldots \in \mathbb{X}$ with $f(\boldsymbol{x}^{(k)}) \to p^*$ as $k \to \infty$. Such a sequence of points is called a minimizing sequence for the minimization problem

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- The algorithm is terminated when $f(\boldsymbol{x}^{(k)}) - p^* \leq \epsilon$, where $\epsilon > 0$ is some specified tolerance

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- The algorithm terminates when $\|\nabla f(\boldsymbol{x}^{(k)})\| \leq \eta$, where η is small and positive
- The above iterative procedure is called a descent method if

$$f(\boldsymbol{x}^{(k+1)}) < f(\boldsymbol{x}^{(k)})$$

except when $\boldsymbol{x}^{(k)}$ is already optimal

Exact line search

- One method for determining the step sizes is exact line search, in which $t^{(k)}$ is chosen to minimize f along the ray $\{\boldsymbol{x}^{(k)} + t\Delta\boldsymbol{x}^{(k)} : t \geq 0\}$:

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- An exact line search is used when the cost of the minimization problem with one variable is low compared to the cost of computing the search direction itself. In some special cases, the minimizer along the ray can be found analytically and in others it can be computed efficiently

Gradient descent

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- A natural choice for the search direction is the negative gradient

$$\Delta \boldsymbol{x}^{(k)} = -\nabla f(\boldsymbol{x}^{(k)})$$

  The resulting algorithm is called the gradient algorithm or gradient descent method

Gradient descent for a quadratic function

- Consider the problem of minimizing

$$f(x_1, x_2) = \frac{1}{2}\left(\sigma_1 x_1^2 + \sigma_2 x_2^2\right)$$

over $\mathbb{R}^2$, where $\sigma_1 \geq \sigma_2 > 0$ are two positive constants

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- Consider gradient descent with exact line search:

$$\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} - t\nabla f(\boldsymbol{x}^{(k)}) = \begin{bmatrix} (1-\sigma_1 t)x_1^{(k)} \\ (1-\sigma_2 t)x_2^{(k)} \end{bmatrix}$$

- Note that

$$f(\boldsymbol{x}^{(k+1)}) = \frac{1}{2}\left[\sigma_1(1-\sigma_1 t)^2(x_1^{(k)})^2 + \sigma_2(1-\sigma_2 t)^2(x_2^{(k)})^2\right]$$

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- Thus, an exact line search yields:

$$t^{(k)} = \frac{\sigma_1^2 (x_1^{(k)})^2 + \sigma_2^2 (x_2^{(k)})^2}{\sigma_1^3 (x_1^{(k)})^2 + \sigma_2^3 (x_2^{(k)})^2}$$

  and hence

$$\boldsymbol{x}^{(k+1)} = \frac{x_1^{(k)} x_2^{(k)} (\sigma_1 - \sigma_2)}{\sigma_1^3 (x_1^{(k)})^2 + \sigma_2^3 (x_2^{(k)})^2} \begin{bmatrix} -\sigma_2^2 x_2^{(k)} \\ \sigma_1^2 x_1^{(k)} \end{bmatrix}$$

- For $k = 0$, we have

$$\boldsymbol{x}^{(1)} = \frac{x_1^{(0)} x_2^{(0)} (\sigma_1 - \sigma_2)}{\sigma_1^3 (x_1^{(0)})^2 + \sigma_2^3 (x_2^{(0)})^2} \begin{bmatrix} -\sigma_2^2 x_2^{(0)} \\ \sigma_1^2 x_1^{(0)} \end{bmatrix}$$

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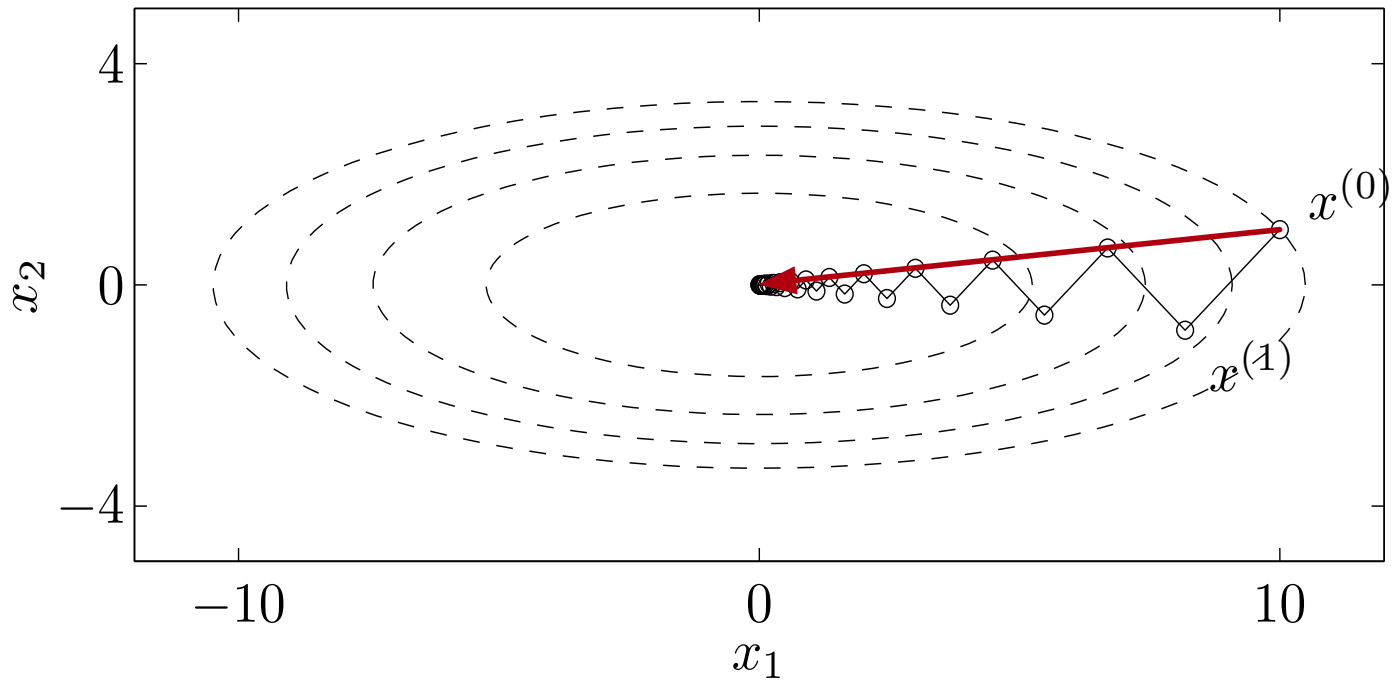
- For $k = 1$, we have

$$\boldsymbol{x}^{(2)} = \frac{x_1^{(1)} x_2^{(1)} (\sigma_1 - \sigma_2)}{\sigma_1^3 (x_1^{(1)})^2 + \sigma_2^3 (x_2^{(1)})^2} \begin{bmatrix} -\sigma_2^2 x_2^{(1)} \\ \sigma_1^2 x_1^{(1)} \end{bmatrix} = \rho \boldsymbol{x}^{(0)}$$

where

$$\rho = \frac{\sigma_1 \sigma_2 (\sigma_1 - \sigma_2)^2 (x_1^{(0)})^2 (x_2^{(0)})^2}{\left[\sigma_1 (x_1^{(0)})^2 + \sigma_2 (x_2^{(0)})^2\right] \left[\sigma_1^3 (x_1^{(0)})^2 + \sigma_2^3 (x_2^{(0)})^2\right]}$$

i.e., for every two iterations we move directly in the line toward the minimum point $\boldsymbol{x}^* = (0, 0)$


4
0
−4
−10
0
10
x_1
x_2
$x^{(0)}$
$x^{(1)}$

- Since f is a quadratic function

$$f(\boldsymbol{x}^{(2)}) - p^* = \rho^2 \left[f(\boldsymbol{x}^{(0)}) - p^* \right]$$

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- Such a convergence behavior is considered to be slow, especially when the ratio ρ (known as convergence rate) is close to 1

- Let $c := \sigma_1/\sigma_2 \geq 1$. The convergence rate

$$\rho = \frac{c(c-1)^2 (x_1^{(0)})^2 (x_2^{(0)})^2}{\left[c(x_1^{(0)})^2 + (x_2^{(0)})^2 \right] \left[c^3 (x_1^{(0)})^2 + (x_2^{(0)})^2 \right]}$$

  is apparently sensitive to the initial point $(x_1^{(0)}, x_2^{(0)})$

- The worse case occurs when $|x_2^{(0)}/x_1^{(0)}| = c$ and in this case, the convergence rate

$$\rho = \left(\frac{c-1}{c+1}\right)^2$$

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- Finally, note here that the Hessian for the quadratic function $f(x_1, x_2) = \frac{1}{2}\left(\sigma_1 x_1^2 + \sigma_2 x_2^2\right)$ is

$$\nabla^2 f = \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix}$$

so σ_1 and σ_2 are the largest and smallest eigenvalue of the Hessian respectively, and ρ is simply the condition number of the Hessian

Gradient descent for strongly convex functions

- For a general objective function f, gradient descent with exact line search is guaranteed to converge if f is strongly convex on its domain, i.e., there exists an $m > 0$ such that

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- Under the strong convexity assumption, it can be shown that

$$f(\boldsymbol{x}^{(k+1)}) - p^* \leq \rho \left[f(\boldsymbol{x}^{(k)}) - p^* \right]$$

where

$$\rho = 1 - \frac{1}{\sup_{\boldsymbol{x} \in \mathrm{dom}(f)} \frac{\lambda_1(\nabla^2 f(\boldsymbol{x}))}{\lambda_n(\nabla^2 f(\boldsymbol{x}))}}$$

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- That is, the gradient method in general exhibits approximately linear convergence, i.e., the optimality gap $f(\boldsymbol{x}^{(k)}) - p^*$ converges to zero approximately as a geometric series

- The convergence rate depends greatly on the condition number of the Hessians. Convergence can be very slow, even for problems that are moderately well conditioned (say, with condition number in the 100s). When the condition number is larger (say, 1000 or more) the gradient method is so slow that it is useless in practice

Steepest descent

- The first-order Taylor approximation of $f(\boldsymbol{x}+\boldsymbol{v})$ around $\boldsymbol{x}$ is

$$f(\boldsymbol{x}+\boldsymbol{v}) \approx f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^t \boldsymbol{v}$$

- The second term on the righthand side, $\nabla f(\boldsymbol{x})^t \boldsymbol{v}$, is the directional derivative of f at $\boldsymbol{x}$ in the direction $\boldsymbol{v}$. It gives the approximate change in f for a small step $\boldsymbol{v}$. The step $\boldsymbol{v}$ is a descent direction if the directional derivative is negative

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- Consider the problem of how to choose $\boldsymbol{v}$ to make the directional derivative as negative as possible. Since the directional derivative $\nabla f(\boldsymbol{x})^t \boldsymbol{v}$ is linear in $\boldsymbol{v}$, it can be made as negative as we like by taking $\boldsymbol{v}$ large (provided $\boldsymbol{v}$ is a descent direction). To make the question sensible we have to limit the length of $\boldsymbol{v}$ or normalize by it

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- Let $\|\cdot\|$ be any norm on $\mathbb{R}^n$. We define a normalized steepest descent direction (with respect to the norm $\|\cdot\|$) as

$$\Delta \boldsymbol{x}_{nsd} = \arg\min\{\nabla f(\boldsymbol{x})^t \boldsymbol{v} : \|\boldsymbol{v}\| = 1\}$$

- It is also convenient to consider a steepest descent step $\Delta \boldsymbol{x}_{sd}$ that is unnormalized, by scaling the normalized steepest descent direction in a particular way:

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- The steepest descent method uses the steepest descent direction as search direction (when exact line search is used, scale factors in the descent direction have no effect, so either normalized or unnormalized direction can be used)

Steepest descent for Euclidean norm

- If we take the norm $\|\cdot\|$ to be the Euclidean norm we find that the steepest descent direction is simply the negative gradient, i.e.,

$$\Delta \boldsymbol{x}_{sd} = -\nabla f(\boldsymbol{x})$$

  Thus, the steepest descent method for the Euclidean norm coincides with the gradient descent method

Steepest descent for quadratic norms

- Consider the quadratic norm

$$\|\boldsymbol{z}\|_{\boldsymbol{P}} = \sqrt{\boldsymbol{z}^t \boldsymbol{P} \boldsymbol{z}} = \|\boldsymbol{P}^{1/2} \boldsymbol{z}\|_2$$

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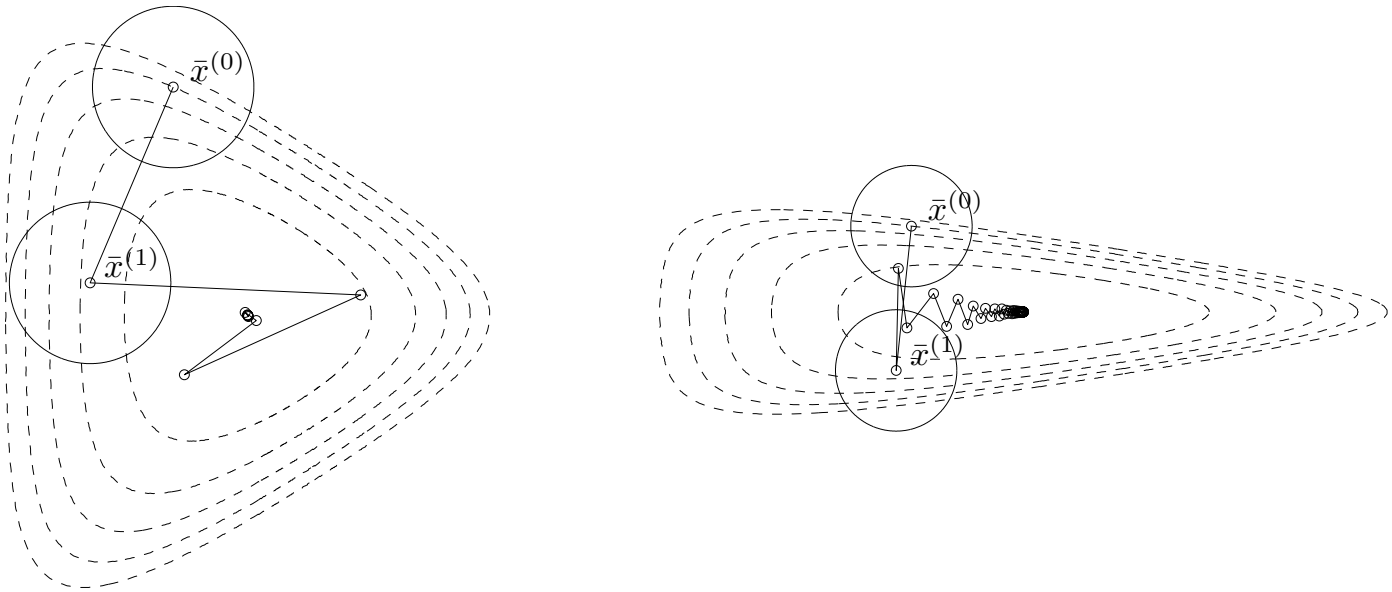
- Alternatively, the steepest descent method in the quadratic norm $\|\cdot\|_{\boldsymbol{P}}$ can be thought of as the gradient method applied to the problem after the change of coordinates

$$\tilde{\boldsymbol{x}} = \boldsymbol{P}^{1/2} \boldsymbol{x}$$



- This observation provides a prescription for choosing $\boldsymbol{P}$: It should be chosen so that the Hessians with respect to $\tilde{\boldsymbol{x}}$ are well conditioned

Steepest descent for ℓ_1-norm

- Consider the steepest descent method for the ℓ_1-norm. It can be shown that a normalized steepest descent direction is given by

$$\Delta \boldsymbol{x}_{nsd} = -\text{sgn}\left(\frac{\partial f(\boldsymbol{x})}{\partial x_{i^*}}\right)\boldsymbol{e}_{i^*}$$

where $i^* = \arg\max_i \left|\frac{\partial f(\boldsymbol{x})}{\partial x_i}\right|$, and $\boldsymbol{e}_i$ is the ith standard basis vector

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- An unnormalized steepest descent step is then

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- Thus, the normalized steepest descent step in ℓ_1-norm can always be chosen to be a standard basis vector (or a negative standard basis vector). It is the coordinate axis direction along which the approximate decrease in f is greatest

Coordinate descent

- The steepest descent algorithm in the ℓ_1 naturally motivates the following coordinate descent algorithm: At each iteration we select a component of $\nabla f(\boldsymbol{x})$ with maximum absolute value, and then decrease or increase the corresponding component of $\boldsymbol{x}$, according to the sign of $(\nabla f(\boldsymbol{x}))_{i^*}$

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- Since only one component of the variable $\boldsymbol{x}$ is updated at each iteration, this can greatly simplify, or even trivialize, the line search
- Consider, for example, the problem:

$$\text{minimize} \quad f(\boldsymbol{x}) = \ln \left(\sum_{i=1}^{n} \sum_{j=1}^{n} M_{i,j}^2 e^{x_i - x_j} \right)$$

- It is easy to minimize f one component at a time. Keeping all components except the kth fixed, we can write

$$f(\boldsymbol{x}) = \ln(\alpha_k + \beta_k e^{-x_k} + \gamma_k e^{x_k})$$

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- The minimum of $f(\boldsymbol{x})$, as a function of x_k, is obtained for

$$x_k = \frac{1}{2} \ln \left(\frac{\beta_k}{\gamma_k} \right)$$

So for this problem an exact line search can be carried out using a simple analytical formula

Convergence analysis

- Similar to gradient descent, it can be shown that for strongly convex functions, steepest descent with exact line search also converges linearly to the minimum point, and the linear convergence rate is again mainly controlled by the condition number of the Hessians

Newton's methods

- The second-order Taylor approximation of $f(\boldsymbol{x}+\boldsymbol{v})$ around $\boldsymbol{x}$ is

$$f(\boldsymbol{x}+\boldsymbol{v}) \approx f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^t \boldsymbol{v} + \frac{1}{2}\boldsymbol{v}^t \nabla^2 f(\boldsymbol{x}) \boldsymbol{v}$$

  which is a convex quadratic function of $\boldsymbol{v}$ and minimized at

$$\boldsymbol{v} = -\nabla^2 f(\boldsymbol{x})^{-1} \nabla f(\boldsymbol{x})$$

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- It is straightforward to verify that

$$\nabla f(\boldsymbol{x})^t \Delta \boldsymbol{x}_{nt} = -\nabla f(\boldsymbol{x})^t \nabla^2 f(\boldsymbol{x})^{-1} \nabla f(\boldsymbol{x}) < 0$$

  unless $\nabla f(\boldsymbol{x}) = \boldsymbol{0}$

- Unfortunately, pure Newton method may not be a descent method. That is, it is possible that $f(\boldsymbol{x}^{(k+1)}) > f(\boldsymbol{x}^{(k)})$, and this may happen if our starting point is far away from the minimum point

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- To overcome the starting-point issue, one may consider using exact line search as opposed to a constant step size $t = 1$. This leads to the so-called damped Newton method

Convergence analysis

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- Finally, we mention that a very important feature of Newton's methods is that it is independent of linear (or affine) changes of coordinates. This is in stark contrast to the gradient (or steepest descent) method, which is strongly affected by changes of coordinates

Backtracking line search

- Most line searches used in practice are inexact: The step length is chosen to approximately minimize f along the ray $\{\boldsymbol{x} + t\Delta\boldsymbol{x} : t \geq 0\}$, or even to just reduce f "enough"

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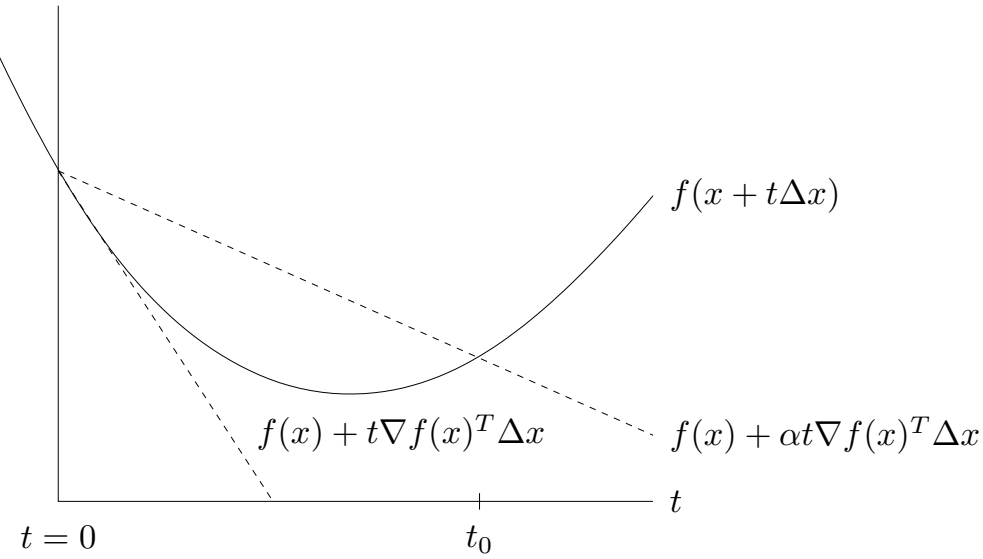
- One inexact line search method that is very simple and quite effective is called backtracking line search. It depends on two constants α and β with $0 < \alpha < 0.5$ and $0 < \beta < 1$
- The line search is called backtracking because it starts with a unit step size and then reduces it by the factor β until the stopping condition

$$f(\boldsymbol{x} + t\Delta\boldsymbol{x}) \leq f(\boldsymbol{x}) + \alpha t \nabla f(\boldsymbol{x})^t \Delta\boldsymbol{x}$$

holds



- Since $\Delta \boldsymbol{x}$ is a descent direction, we have $\nabla f(\boldsymbol{x})^t \Delta \boldsymbol{x} < 0$, so for small enough t we have

$$f(\boldsymbol{x} + t\Delta \boldsymbol{x}) \approx f(\boldsymbol{x}) + t\Delta f(\boldsymbol{x})^t \Delta \boldsymbol{x} < f(\boldsymbol{x}) + \alpha t \Delta f(\boldsymbol{x})^t \Delta \boldsymbol{x}$$

  which shows that the backtracking line search eventually terminates. The constant α can be interpreted as the fraction of the decrease in f predicted by linear extrapolation that we will accept