MS-E2122 - Nonlinear Optimization
Lecture V

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Outline of this lecture

Line search methods - univariate (single variable) optimisation

- Line searches without derivatives
- Line searches with derivatives

Methods for unconstrained optimisation

- Coordinate descent
- Gradient method
- Newton's method

- Optimality conditions;
- KKT conditions

Outline of this lecture

Line search methods

This pseudocode represents the general concept of optimization methods:

Algorithm Conceptual optimisation algorithm

```
initialise. iteration count k = 0, starting point x_0
while stopping criteria are not met do
    compute direction d_k
    compute step size λ_k
    x_{k+1} = x_k + λ_k d_k
    k = k + 1
end while
return x_k
```

where

- k is an iteration counter;
- λ_k is a suitable step size;
- d_k is a direction vector;

Line search methods

Finding an optimal step size λ_k is in itself an optimisation problem called line search due to its **unidimensional** nature.

Line searches are the backbone of most optimisation methods.

Let $\theta(\lambda) = f(x + \lambda d)$. If f is **differentiable**, a straightforward approach is to find an optimal setup size λ is

$$\theta'(\lambda) = d^\top \nabla f(x + \lambda d) = 0$$

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$$\theta'(\lambda) = d^\top \nabla f(x + \lambda d) = 0$$

However, one must bear in mind that:

- $d^\top f(x + \lambda d)$ is often nonlinear in λ;
- $\overline{\lambda} = \mathrm{argmin}_\lambda\, d^\top \nabla f(x + \lambda d) = 0$ is not necessarily optimal.

Line search methods

Theorem 1 (Line search reduction)

Let $\theta : \mathbb{R} \to \mathbb{R}$ *be strictly quasiconvex over the interval* $[a, b]$*, and let* $\lambda, \mu \in [a, b]$ *such that* $\lambda < \mu$*. If* $\theta(\lambda) > \theta(\mu)$*, then* $\theta(z) \geq \theta(\mu)$ *for all* $z \in [a, \lambda]$*. If* $\theta(\lambda) \leq \theta(\mu)$*, then* $\theta(z) \geq \theta(\lambda)$ *for all* $z \in [\mu, b]$*.*

Line search methods

Theorem 1 (Line search reduction)

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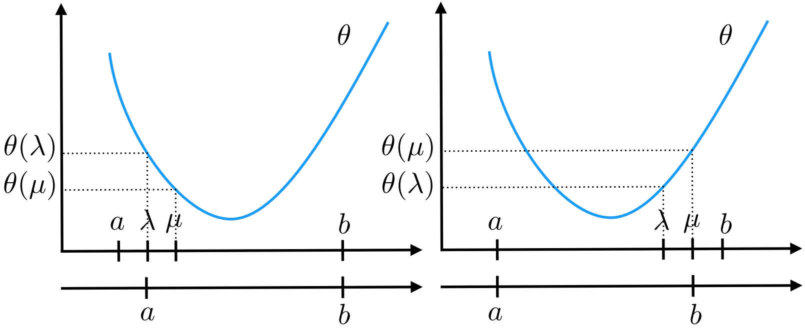

Applying Theorem 1 allows to iteratively reduce the search space.

Line search methods - uniform search

Break $[a, b]$ into n uniform intervals of size δ, which leads to $n + 1$ grid points $a_k = a_0 + k\delta$, with $a = a_0, b = a_n$, and $k = 0, \ldots, n$.

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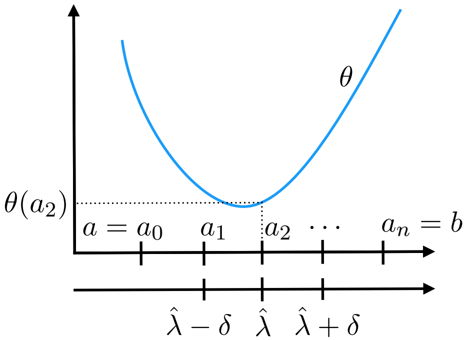

Grid search with 5 points; Note that $\theta(a_2) = \min_{i=0,\dots,n} \theta(a_i)$.

Let $\hat{\lambda} = \operatorname{argmin}_{i=0,\dots,n} \theta(a_i)$.
We know that the optimal $\overline{\lambda} \in [\hat{\lambda} - \delta, \hat{\lambda} + \delta]$.

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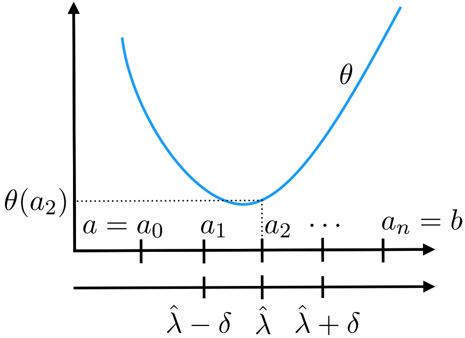

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Remarks:

- The search can be repeated making $a = \hat{\lambda} - \delta$ and $b = \hat{\lambda} + \delta$.
- The number of grid points can increase dynamically, saving function evaluations.

Line search methods - sequential searches

More efficient methods can be devised by using information of the **previous** evaluation of θ. These are known as sequential searches.

1. Dichotomous search: we place two points, λ and μ, around the midpoint of $[a, b]$ at a small distance ϵ.

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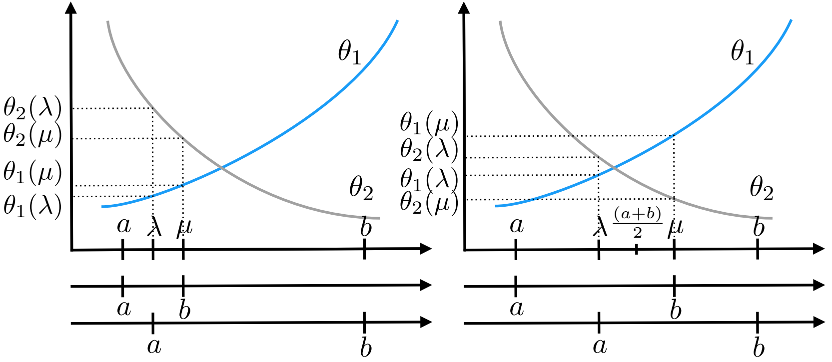

Using the midpoint $(a + b)/2$ and Theorem 1 to reduce the search space.

Line search methods - sequential searches

Algorithm Dichotomous search

initialise. distance $\epsilon > 0$, tolerance $l > 0$, $[a_0, b_0] = [a, b]$, $k = 0$
while $b_k - a_k > l$ **do**
  $\lambda_k = \frac{a_k+b_k}{2} - \epsilon$, $\mu_k = \frac{a_k+b_k}{2} + \epsilon$
  if $\theta(\lambda_k) < \theta(\mu_k)$ **then**
    $a_{k+1} = a_k$, $b_{k+1} = \mu_k$
  else
    $a_{k+1} = \lambda_k$, $b_{k+1} = b_k$
  end if
  $k = k + 1$
end while
return $\overline{\lambda} = \frac{a_k+b_k}{2}$

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Remark: The number of steps (and evaluations of θ) can be predicted beforehand:

$$b_{k+1} - a_{k+1} = \frac{1}{2^k}(b_0 - a_0) + 2\epsilon\left(1 - \frac{1}{2^k}\right).$$

Bisection method

More than just function evaluations, it also uses derivative information. We assume $\theta(\lambda)$ to be **differentiable** and **convex**.

2. Bisection method: The main idea is

1. if $\theta'(\lambda_k) = 0$, then λ_k is a **minimiser**.

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2. if $\theta'(\lambda_k) > 0$, then, for $\lambda > \lambda_k$, we have $\theta'(\lambda_k)(\lambda - \lambda_k) \geq 0$, which implies $\theta(\lambda) \geq \theta(\lambda_k)$ since θ is **convex**. Therefore, the new search interval becomes $[a_{k+1}, b_{k+1}] = [a_k, \lambda_k]$.

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   3. if $\theta'(\lambda_k) < 0$, we have $\theta'(\lambda_k)(\lambda - \lambda_k) \geq 0$ for $\lambda < \lambda_k$. Thus, the new search interval becomes $[\boldsymbol{a_{k+1}}, \boldsymbol{b_{k+1}}] = [\boldsymbol{\lambda_k}, \boldsymbol{b_k}]$.

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4. As in the dichotomous search, to maximise overall interval reduction, we set $\lambda_k = \frac{1}{2}(b_k + a_k)$.

Bisection method

Algorithm Bisection method

initialise. tolerance $l > 0$, $[a_0, b_0] = [a, b]$, $k = 0$
while $b_k - a_k > l$ **do**
  $\lambda_k = \frac{(b_k + a_k)}{2}$ and evaluate $\theta'(\lambda_k)$
  if $\theta'(\lambda_k) = 0$ **then** return λ_k
  else if $\theta'(\lambda_k) > 0$ **then**
    $a_{k+1} = a_k,\ b_{k+1} = \lambda_k$
  else
    $a_{k+1} = \lambda_k,\ b_{k+1} = b_k$
  end if
  $k = k + 1.$
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return $\overline{\lambda} = \frac{a_k + b_k}{2}$

Inexact line searches - Armijo rule

Often the use of non-optimal (i.e., inexact) step sizes λ_k is enough to guarantee a good performance.

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$$f(\overline{x} + d\overline{\lambda}) - f(\overline{x}) \leq \alpha\overline{\lambda}\nabla f(\overline{x})^\top d$$

which, at $\lambda = 0$, is the same as

$$\begin{aligned} &\theta(\overline{\lambda}) - \theta(0) \leq \alpha\overline{\lambda}\theta'(0) \\ &\theta(\overline{\lambda}) \leq \theta(0) + \alpha\overline{\lambda}\theta'(0) : \text{ Armijo's rule (AR)} \end{aligned}$$

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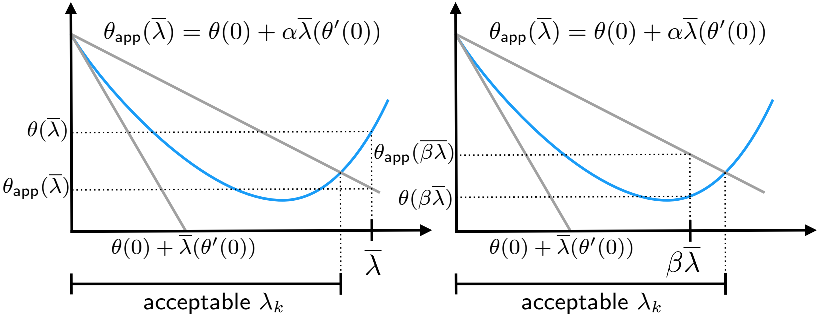
$$\theta(\overline{\lambda}) \leq \theta(0) + \alpha\overline{\lambda}\theta'(0) : \text{ Armijo's rule (AR)}$$

If $\overline{\lambda}$ does not satisfy AR, $\overline{\lambda}$ is reduced by a factor $\beta \in (0, 1)$ and the test is repeated until (AR) is satisfied.

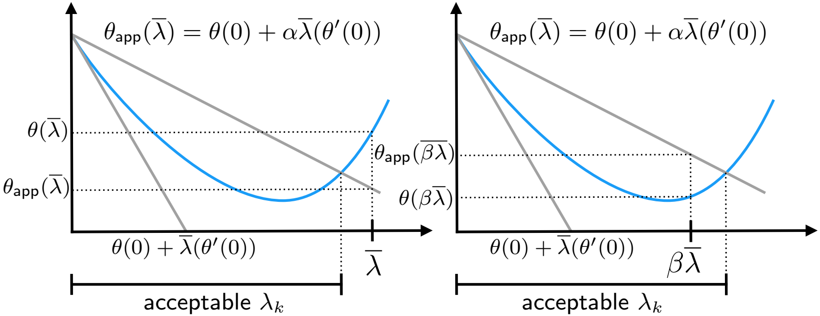
Inexact line searches - Armijo's rule

Armijo's rule has a nice graphical interpretation: $\overline{\lambda}$ is accepted if it is in an interval where the function $\theta(\lambda)$ is below a deflected linear extrapolation (from 0).



At first $\lambda_0 = \overline{\lambda}$ is not acceptable; after reducing the step size to $\lambda_1 = \beta\overline{\lambda}$, it enters the acceptable range where $\theta(\lambda_k) \leq \theta_{\text{app}}(\lambda_k) = \theta(0) + \alpha\lambda_k(\theta'(0))$.

Inexact line searches - Armijo's rule



Remarks:

1. Some variants also consider rules to guarantee that $\overline{\lambda}$ is not too small, such as $\theta(\delta\overline{\lambda}) \leq \theta(0) + \alpha\delta\overline{\lambda}\theta'(0)$, with $\delta > 1$.
2. Also known in the literature as backtracking.
3. Typical values: $\alpha \in [0.1, 0.5]$ and $\beta \in [0.6, 0.99]$. Very small α, e.g. 10^{-4} is often used as well.

Outline of this lecture

Coordinate descent

Next, we focus on optimizing functions $f : \mathbb{R}^n \to \mathbb{R}$ with **more** than one dimension.

The main difference is that we need to specify search directions d at each point $x \in \mathbb{R}^n$.

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1. Coordinate descent: the search direction is one coordinate axis per iteration. That is, $d_i = 1$ for coordinate i and $d_{j \neq i} = 0$, for $i, j \in \{1, \ldots, n\}$.

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Several variants:

1. **Cyclic:** coordinates are considered in order $1, \ldots, n$;
2. **Double-sweep:** swap the coordinate order at each iteration;
3. **Gauss-Southwell:** choose components with largest $\frac{\partial f(x)}{\partial x_i}$;
4. **Stochastic:** coordinates are selected at random

Coordinate descent

Algorithm Coordinate descent method (cyclic)

initialise. tolerance $\epsilon > 0$, initial point x^0, iteration count $k = 0$
while $||x^{k+1} - x^k|| > \epsilon$ **do**
  for $j = 1, \dots n$ **do**
    $d = \{d_i = 1, \text{ if } i = j; d_i = 0, \text{ if } i \neq j\}$
    $\overline{\lambda}_j = \text{argmin}_{\lambda \in \mathbb{R}} \left\{ f(x_j^k + \lambda d_j) \right\}$
    $x_j^{k+1} = x_j^k + \overline{\lambda}_j d_j$
  end for
  $k = k + 1$
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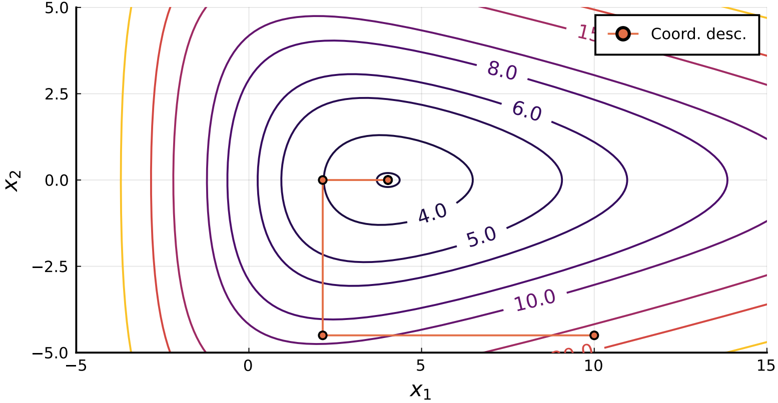
Remarks:

1. The one-dimensional minimisation is called Gauss-Seidel step;
2. Block-coordinate methods use subgroups (blocks) of coordinates to define directions.

Coordinate descent

$$f(x) = e^{(-(x_1-3)/2)} + e^{((4x_2+x_1)/10)} + e^{((-4x_2+x_1)/10)}$$



Coordinate descent method applied to f. Convergence is observed in 4 steps for a tolerance $\epsilon = 10^{-4}$

Gradient method

Recall that if d is a **descent direction**, there exists $\delta > 0$ such that $f(x + \lambda d) < f(x)$ for all $\lambda \in (0, \delta)$. The following result provides directions of steepest descent.

Lemma 2 (Steepest descent direction)

Suppose that $f : \mathbb{R}^n \to \mathbb{R}$ *is differentiable at* $x \in \mathbb{R}^n$ *and* $\nabla f(x) \neq 0$. *Then* $\overline{d} = -\frac{\nabla f(x)}{||\nabla f(x)||}$ *is the direction of steepest descent of* f *at* x.

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Proof.

From differentiability of f, we have

$$f'(x; d) = \lim_{\lambda \to 0^+} \frac{f(x + \lambda d) - f(x)}{\lambda} = \nabla f(x)^\top d.$$

Thus, $\overline{d} = \operatorname{argmin}_{||d|| \leq 1} \left\{ \nabla f(x)^\top d \right\} = -\frac{\nabla f(x)}{||\nabla f(x)||}$. $\square$

Gradient method

Algorithm Gradient method

1: **initialise.** tolerance $\epsilon > 0$, initial point x_0, iteration count $k = 0$.
2: **while** $||\nabla f(x_k)|| > \epsilon$ **do**
3: $\quad d = -\frac{\nabla f(x_k)}{||\nabla f(\overline{x})||}$
4: $\quad \overline{\lambda} = \text{argmin}_{\lambda \in \mathbb{R}} \{f(x_k + \lambda d)\}$
5: $\quad x_{k+1} = x_k + \overline{\lambda} d_j$
6: $\quad k = k + 1$
7: **end while**
8: **return** x_k

Gradient method

Algorithm Gradient method

```
initialise. tolerance ϵ > 0, initial point x_0, iteration count k = 0.
while ||∇f(x_k)|| > ϵ do
    d = −∇f(x_k) / ||∇f(x̄)||
    λ̄ = argmin_{λ∈ℝ} {f(x_k + λd)}
    x_{k+1} = x_k + λ̄ d_j
    k = k + 1
end while
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```

Remarks:

1. Steepest descent and gradient methods are different. When $||d|| \leq 1$ uses 2-norm (in Lemma 2), they are equivalent;

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Remarks:

1. Steepest descent and gradient methods are different. When $||d|| \leq 1$ uses 2-norm (in Lemma 2), they are equivalent;
2. Poor convergence and zigzagging can be observed due to imprecise linear approximations (more on this later);

Gradient method

$$f(x) = e^{(-(x_1-3)/2)} + e^{((4x_2+x_1)/10)} + e^{((-4x_2+x_1)/10)}$$

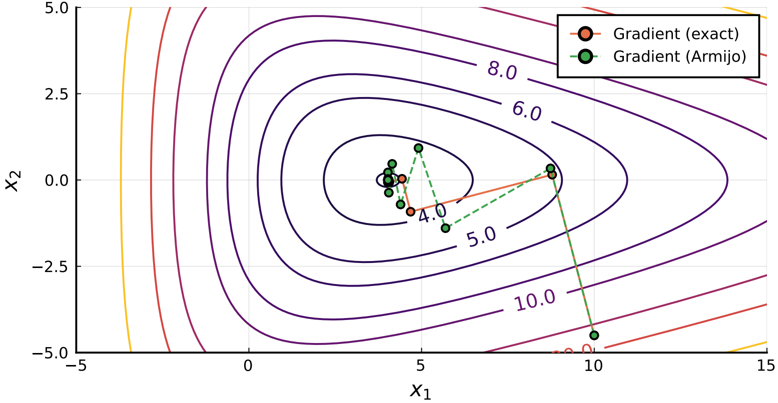

Figure: Gradient method applied to f. Convergence is observed in 9 steps using exact line search and 15 using Armijo's rule ($\epsilon = 10^{-4}$)

Newton's method

Same idea as in the **univariate** case. Can also be seen as deflected steepest descent.

Deflection is achieved using the Hessian, which is equivalent to relying on quadratic approximations (rather than linear).

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Consider the 2$^{\text{nd}}$-order approximation of f at x_k:

$$q(x) = f(x_k) + \nabla f(x_k)^\top (x - x_k) + \frac{1}{2}(x - x_k)^\top H(x_k)(x - x_k),$$

where $H(x_k)$ is the Hessian at x_k.

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where $H(x_k)$ is the Hessian at x_k. We require that $\nabla q(x_{k+1}) = 0$, which leads to

$$\nabla f(x_k) + H(x_k)(x - x_k) = 0.$$

Assuming that $H^{-1}(x_k)$ exists, we obtain the update rule

$$x_{k+1} = x_k - H^{-1}(x_k)\nabla f(x_k).$$

Newton's method

Algorithm Newton's method

initialise. tolerance $\epsilon > 0$, initial point x_0, iteration count $k = 0$
while $||\nabla f(x_k)|| > \epsilon$ **do**
    $d = -H^{-1}(x_k)\nabla f(x_k)$
    $\overline{\lambda} = \text{argmin}_{\lambda \in \mathbb{R}} \{f(x_k + \lambda d)\}$
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Remarks:

1. Setting $\overline{\lambda} = 1$ recovers the "pure" Newton's method;
2. As $\nabla f(x_k)$ gets close to 0, $H^{-1}(x_k)$ becomes singular;
3. It might not converge if x_0 is too far from optimal and fixed step size is used;

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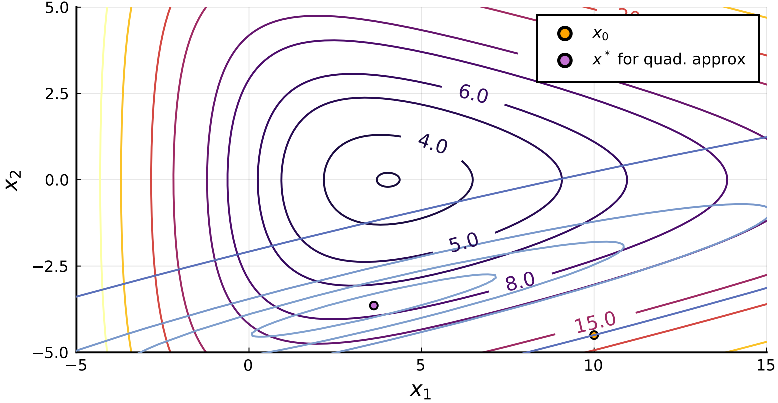
2: **while** $||\nabla f(x_k)|| > \epsilon$ **do**
3: $\quad d = -H^{-1}(x_k)\nabla f(x_k)$
4: $\quad \overline{\lambda} = \text{argmin}_{\lambda \in \mathbb{R}} \{f(x_k + \lambda d)\}$
5: $\quad x_{k+1} = x_k + \overline{\lambda} d$
6: $\quad k = k + 1$
7: **end while**
8: **return** x_k

Remarks:

1. Setting $\overline{\lambda} = 1$ recovers the "pure" Newton's method;
2. As $\nabla f(x_k)$ gets close to 0, $H^{-1}(x_k)$ becomes singular;
3. It might not converge if x_0 is too far from optimal and fixed step size is used;
4. Levenberg-Marquardt method and other trust-region method variants also address convergence issues of Newton's method.

Newton's method

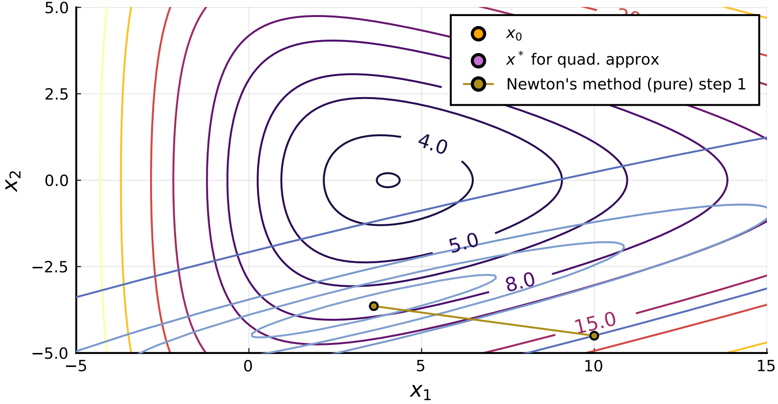
$$f(x) = e^{(-(x_1-3)/2)} + e^{((4x_2+x_1)/10)} + e^{((-4x_2+x_1)/10)}$$



The quadratic approximation at x_0 (with level curves in blue) and the optimal point x^*.

Newton's method

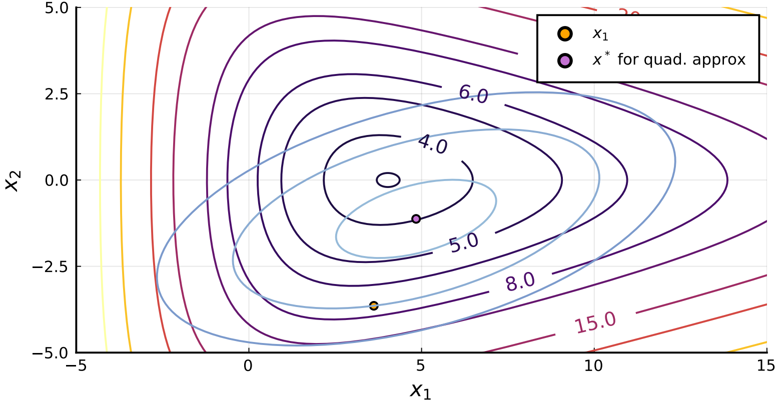
$$f(x) = e^{(-(x_1-3)/2)} + e^{((4x_2+x_1)/10)} + e^{((-4x_2+x_1)/10)}$$



The new point x_1 becomes x^*.

Newton's method

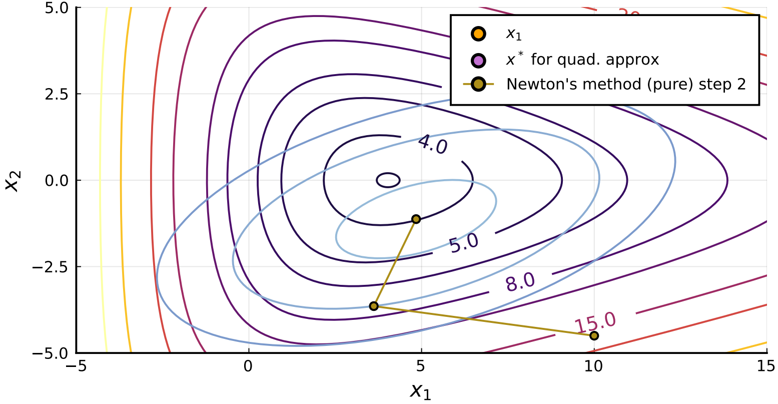
$$f(x) = e^{(-(x_1-3)/2)} + e^{((4x_2+x_1)/10)} + e^{((-4x_2+x_1)/10)}$$



The new quadratic approximation at x_1 and new optimal point x^*. Notice how the approximation improved.

Newton's method

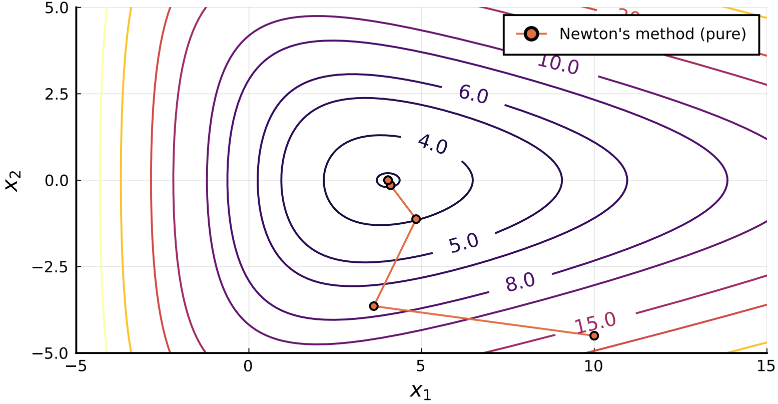
$$f(x) = e^{(-(x_1-3)/2)} + e^{((4x_2+x_1)/10)} + e^{((-4x_2+x_1)/10)}$$



The new point x_2 becomes x^*.

Newton's method

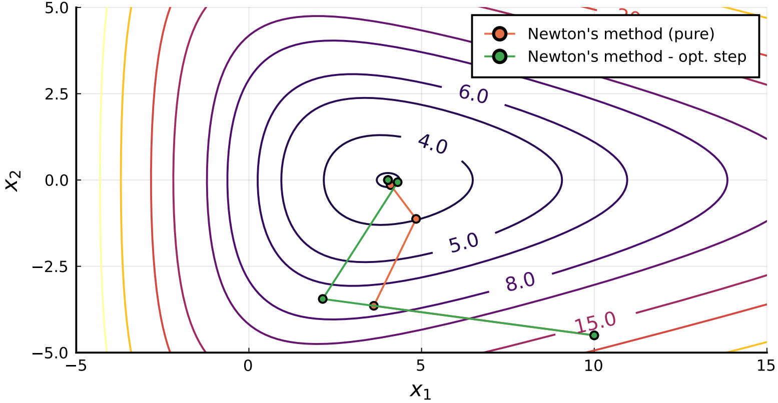
$$f(x) = e^{(-(x_1-3)/2)} + e^{((4x_2+x_1)/10)} + e^{((-4x_2+x_1)/10)}$$



The complete trajectory of the pure Newton's method.

Newton's method

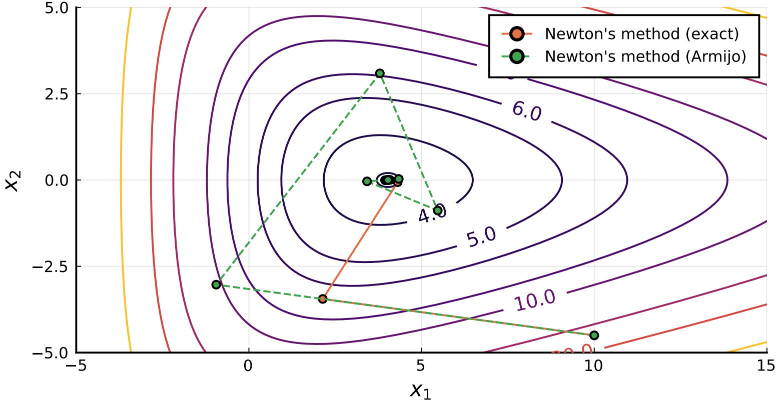
$$f(x) = e^{(-(x_1-3)/2)} + e^{((4x_2+x_1)/10)} + e^{((-4x_2+x_1)/10)}$$



When employing line searches, the direction $x_k - x_{k-1}$ from the pure method is used, but the actual step is optimised.

Newton's method

$$f(x) = e^{(-(x_1-3)/2)} + e^{((4x_2+x_1)/10)} + e^{((-4x_2+x_1)/10)}$$



Newton's method applied to f. Convergence is observed in 4 steps using exact line search and 27 using Armijo's rule ($\epsilon = 10^{-4}$)


THANK YOU