Optimisation Methods II

Matteo Fasiolo

Recap on SD and Newton's methods

Weaknesses of steepest descent:

- Provides direction but no information on step-length;
- Tends to zig-zag.

Improved by Newton's method via a better local model, but:

1. Needs to compute the Hessian matrix $\mathbf{H}$;
2. Need to ensure its positive definiteness.

Both need line search to guarantee convergence.

Can we avoid having to derive and compute $\mathbf{H}$?

Obvious solution is to approximate $\mathbf{H}$ via finite differences (FD).

This remove analytical effort, but still need to store $\mathbf{H}$ and solve:

$$\mathbf{H}\boldsymbol{\Delta} = -\nabla f(\boldsymbol{\theta}).$$

FD can be expensive: $p = \dim(\boldsymbol{\theta})$ gradient evaluations needed.

Alternative is to use **quasi-Newton** methods.

Idea is to use past gradients to update an approximate Hessian.

Update can be performed:

- Directly on inverse $\mathbf{B} = \mathbf{H}^{-1}$ so we can compute

$$\boldsymbol{\Delta} = -\mathbf{H}^{-1}\nabla f(\boldsymbol{\theta}) = -\mathbf{B}\nabla f(\boldsymbol{\theta}).$$

- So to guarantee that $\mathbf{B}$ is positive definite.

Quasi-Newton methods

At $\boldsymbol{\theta}^{[k]}$ we have pos. def. approx. to $\mathbf{H}^{[k]}$ and $\mathbf{B}^{[k]}$.

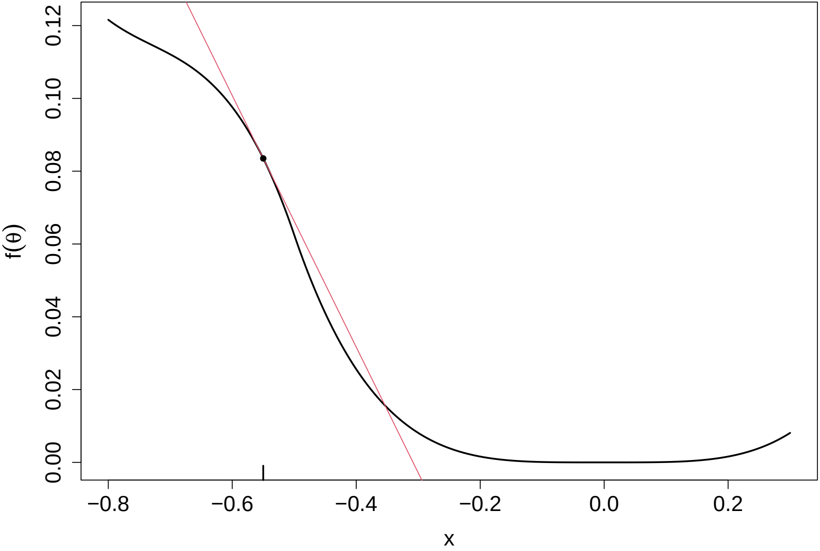
So search direction is

$$\boldsymbol{\Delta} = -\mathbf{B}^{[k]} \nabla f(\boldsymbol{\theta}^{[k]})$$

Along the $\boldsymbol{\theta}^{[k]} + \boldsymbol{\Delta}$ direction we can evaluate $f(\boldsymbol{\theta})$ and $\nabla f(\boldsymbol{\theta})$.

How to use them to update to (pos. def.) $\mathbf{H}^{[k+1]}$ and $\mathbf{B}^{[k+1]}$?

To get intuition, consider 1D case.



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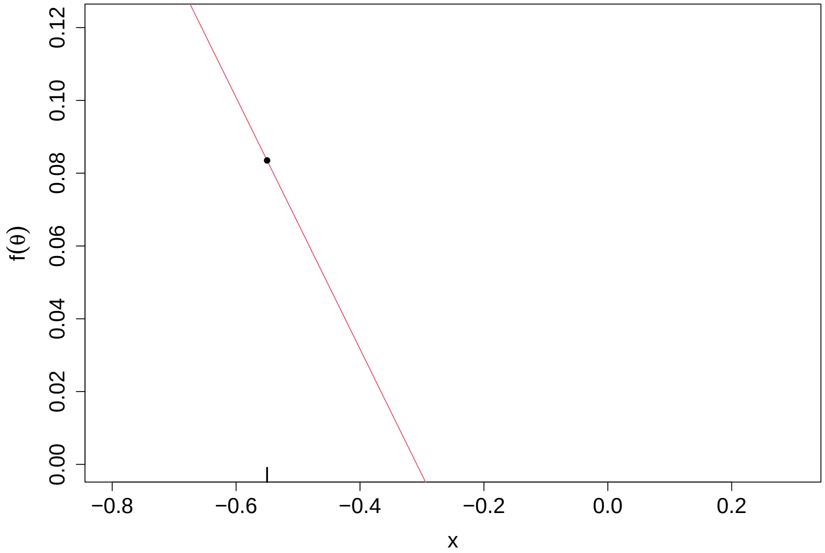

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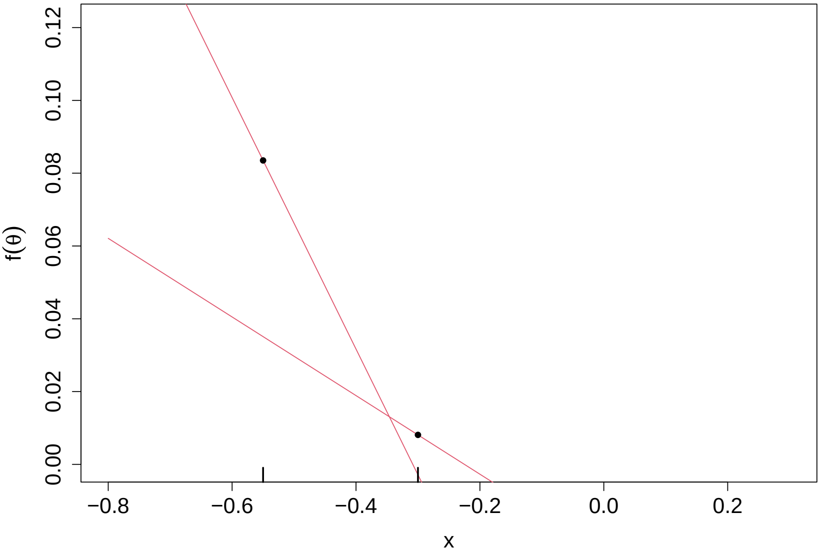

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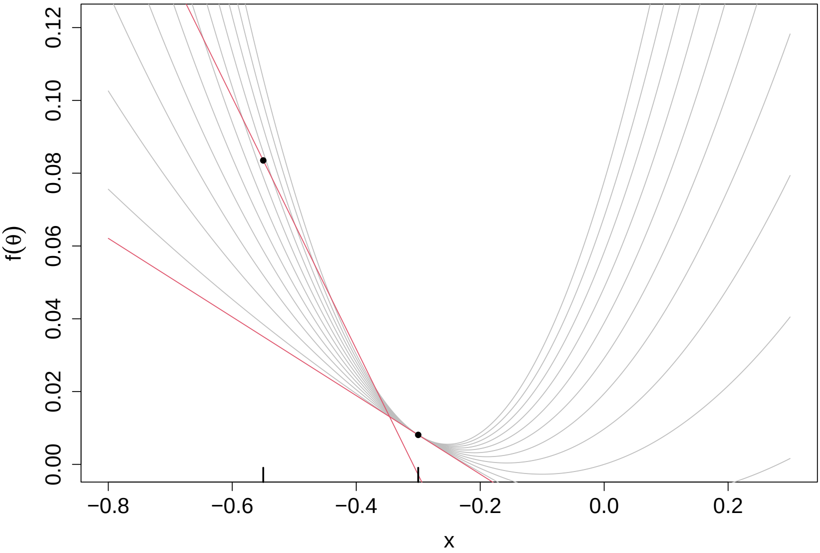

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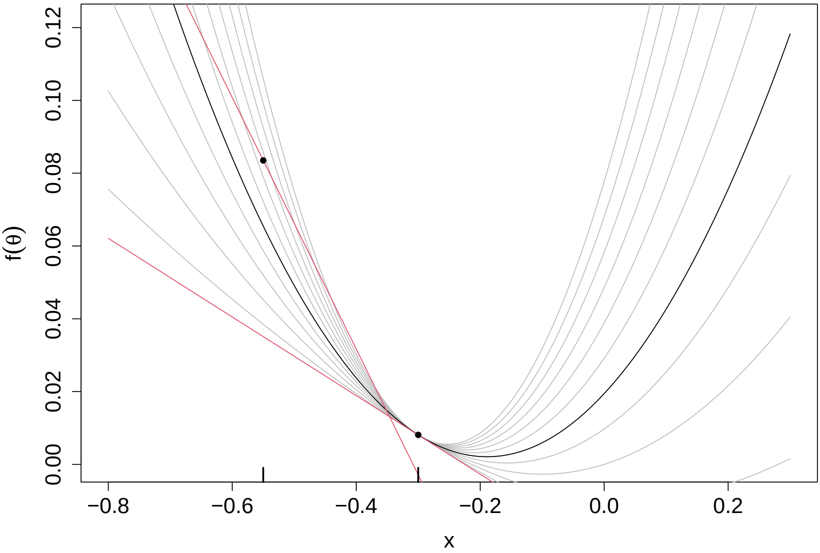

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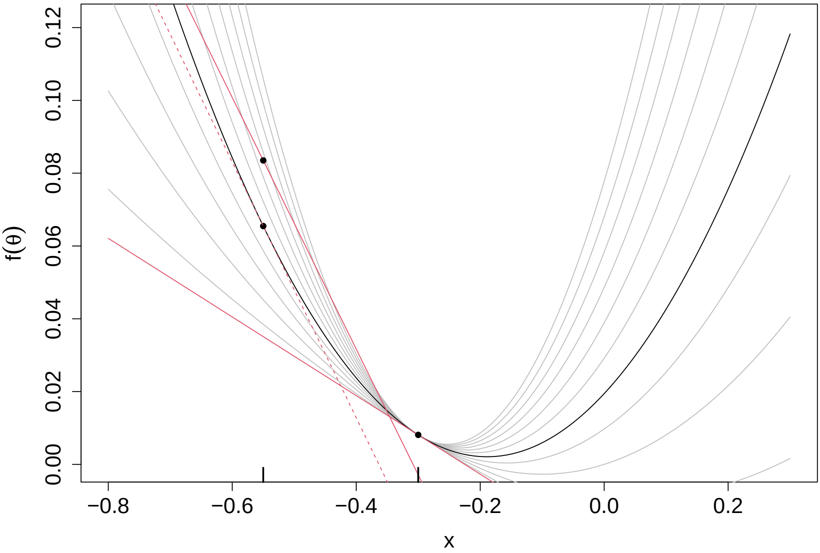


What are we doing? Let $f'(\theta)$ be $\frac{df}{d\theta}$.

We considered the local model at $\theta^{[k+1]}$

$$f(\theta) \simeq \tilde{f}(\theta) = f(\theta^{[k+1]}) + f'(\theta^{[k+1]})(\theta - \theta^{[k+1]}) + \frac{1}{2} H (\theta - \theta^{[k+1]})^2,$$

we differentiate w.r.t. θ

$$\tilde{f}'(\theta) = f'(\theta^{[k+1]}) + H(\theta - \theta^{[k+1]}),$$

and find H such that $f'(\theta^{[k]}) = \tilde{f}'(\theta^{[k]})$, that is

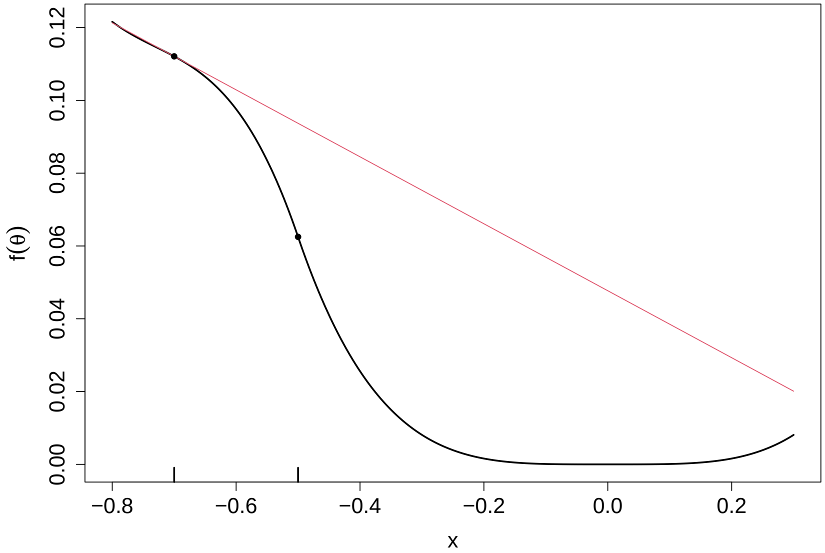
$$f'(\theta^{[k]}) = f'(\theta^{[k+1]}) + H(\theta^{[k]} - \theta^{[k+1]}),$$

so (anticlimax here)

$$H^{[k+1]} = \frac{f'(\theta^{[k+1]}) - f'(\theta^{[k]})}{\theta^{[k+1]} - \theta^{[k]}} \quad \text{(finite differences, not updating } H^{[k]}\text{)}$$

But $H > 0$ implies that if $\theta^{[k+1]} > \theta^{[k]}$ then $f'(\theta^{[k+1]}) > f'(\theta^{[k]})$.

This is not always the case:



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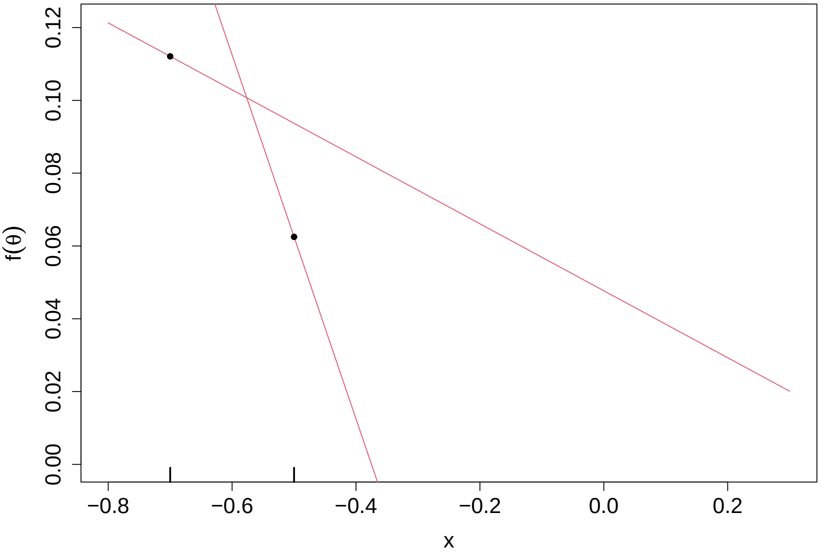

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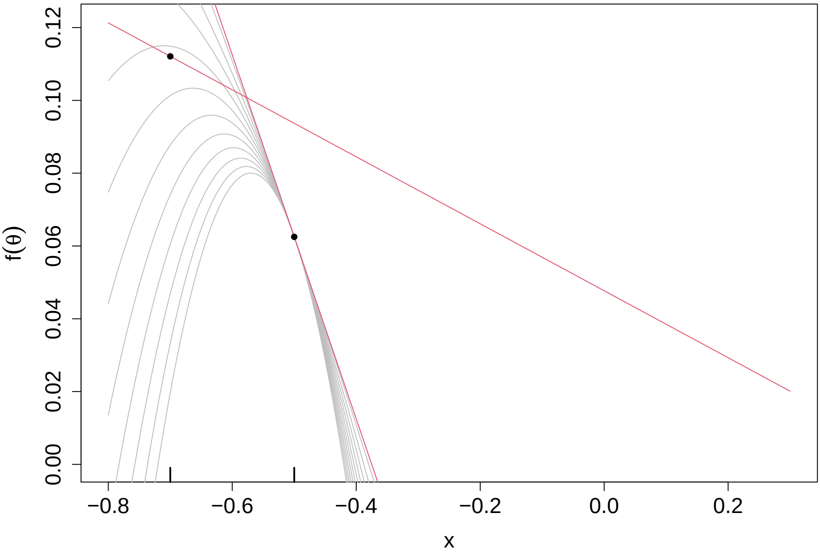

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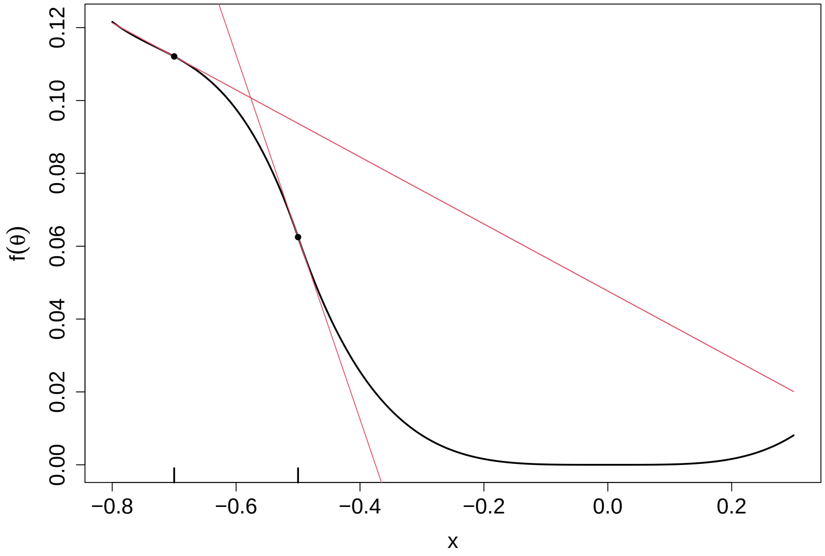

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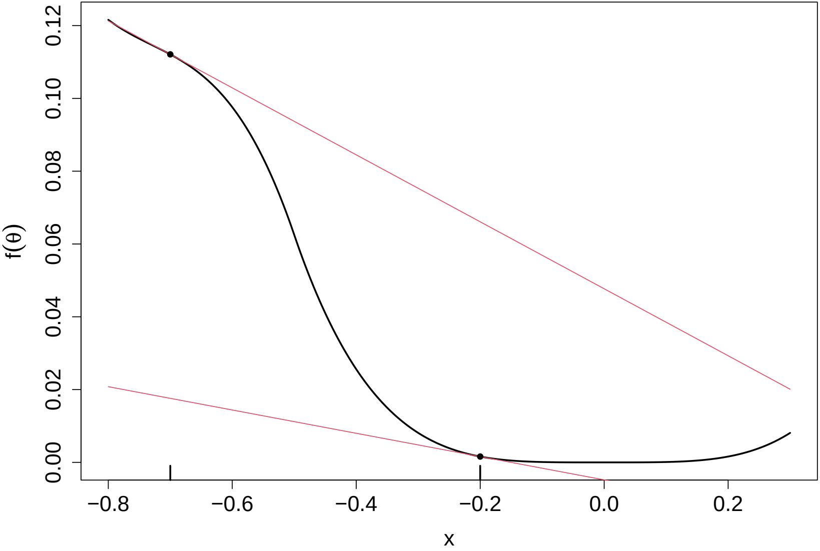

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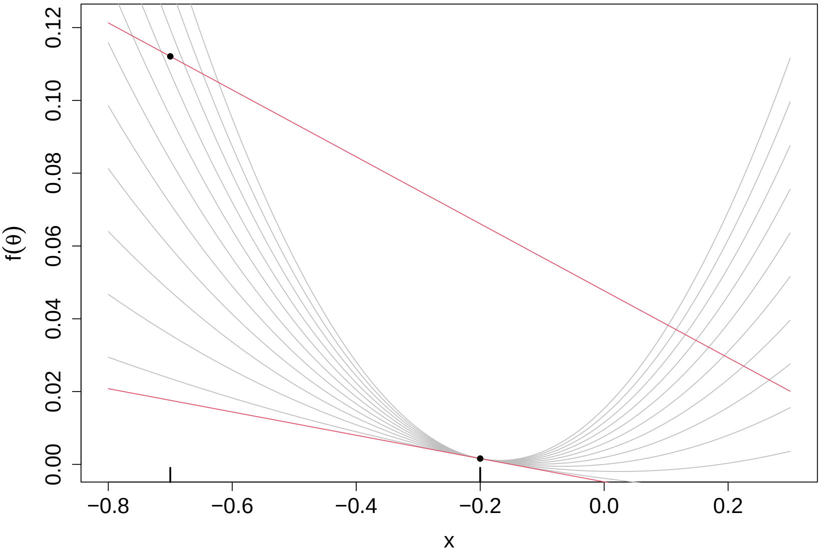

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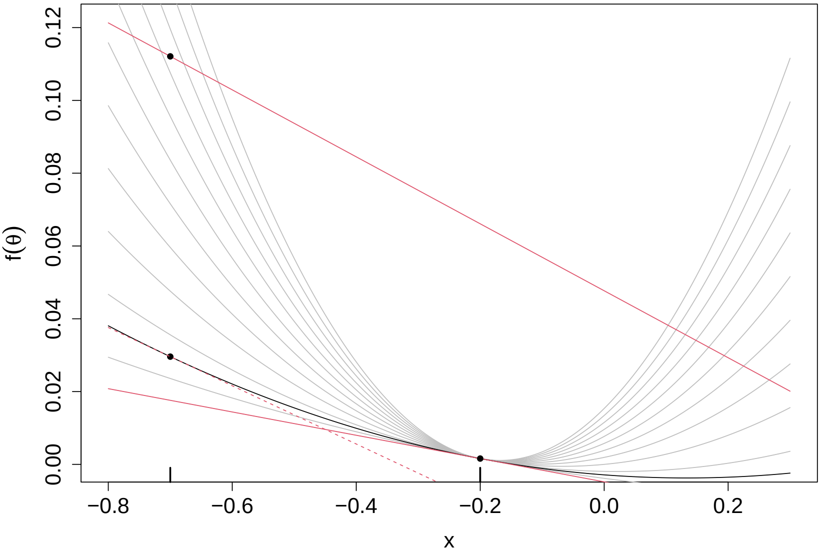


In $\mathrm{D} > 1$ "gradient matching requirement" (**secant equation**) is

$$\nabla f(\boldsymbol{\theta}^{[k]}) = \nabla f(\boldsymbol{\theta}^{[k+1]}) + \mathbf{H}^{[k+1]}(\boldsymbol{\theta}^{[k]} - \boldsymbol{\theta}^{[k+1]}).$$

Rearranging

$$\nabla f(\boldsymbol{\theta}^{[k+1]}) - \nabla f(\boldsymbol{\theta}^{[k]}) = \mathbf{H}^{[k+1]}(\boldsymbol{\theta}^{[k+1]} - \boldsymbol{\theta}^{[k]}),$$

or $\mathbf{B}^{[k+1]}\mathbf{y}_k = \mathbf{s}_k$.

$\mathbf{H}^{[k+1]}$ has p^2 elements but equation imposes p constraints.

So it does not uniquely define $\mathbf{H}^{[k+1]}$ or its update from $\mathbf{H}^{[k]}$.

The BFGS method finds the update that solves

$$\mathbf{B}^{[k+1]} = \underset{\mathbf{B}}{\operatorname{argmin}} ||\mathbf{B} - \mathbf{B}^{[k]}||_{\mathrm{Frob}},$$

subject to

$$\mathbf{B} = \mathbf{B}^{\mathsf{T}} \quad \text{and} \quad \mathbf{B}\mathbf{y}_k = \mathbf{s}_k.$$

But there are other options, e.g. the DFP update for $\mathbf{H}^{[k+1]}$.

The solution to constrained optimisation problem is:

$$\mathbf{B}^{[k+1]} = (\mathbf{I} - \rho_k \mathbf{s}_k \mathbf{y}_k^\mathsf{T}) \mathbf{B}^{[k]} (\mathbf{I} - \rho_k \mathbf{y}_k \mathbf{s}_k^\mathsf{T}) + \rho_k \mathbf{s}_k \mathbf{s}_k^\mathsf{T}$$

where $\rho_k^{-1} = \mathbf{s}_k^\mathsf{T} \mathbf{y}_k$, or

$$\mathbf{B}^{[k+1]} = \mathbf{B}^{[k]} + \rho_k \mathbf{s}_k \mathbf{y}_k^\mathsf{T} \mathbf{B}^{[k]} \left(\rho_k \mathbf{y}_k \mathbf{s}_k^\mathsf{T} - 2\mathbf{I} \right) + \rho_k \mathbf{s}_k \mathbf{s}_k^\mathsf{T}$$

which is a rank-2 update.

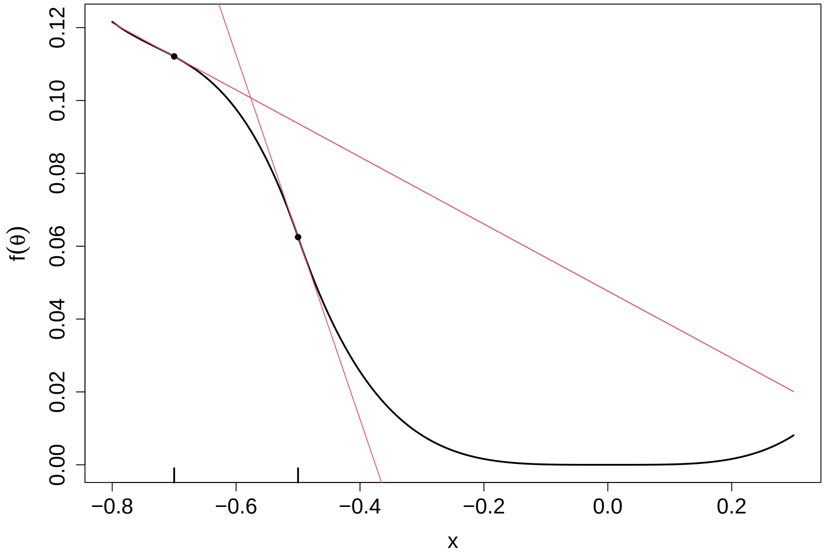
Note: we did not impose positive definiteness constraint on $\mathbf{B}^{[k+1]}$.

This is guaranteed if

$$\rho_k^{-1} = (\boldsymbol{\theta}^{[k+1]} - \boldsymbol{\theta}^{[k]})^\mathsf{T} (\nabla f(\boldsymbol{\theta}^{[k+1]}) - \nabla f(\boldsymbol{\theta}^{[k]})) > 0.$$

You want $f(\boldsymbol{\theta})$ to become flatter in the direction of the step.

Here ρ_k would be negative:



$\rho_k > 0$ ensured by step-length α statisfying **Wolf conditions**.

Recall step is $\boldsymbol{\Delta}_\alpha = \alpha\boldsymbol{\Delta} = -\alpha\mathbf{B}^{[k]}\nabla f(\boldsymbol{\theta}^{[k]})$.

Recall $\nabla f(\boldsymbol{\theta}^{[k]})^\mathsf{T}\boldsymbol{\Delta}_\alpha < 0$ if $\mathbf{B}^{[k]}$ is pos def.

First is **sufficient decrease** condition:

$$f(\boldsymbol{\theta}^{[k]} + \boldsymbol{\Delta}_\alpha) \leq f(\boldsymbol{\theta}^{[k]}) + c_1\nabla f(\boldsymbol{\theta}^{[k]})^\mathsf{T}\boldsymbol{\Delta}_\alpha$$

with $c_1 \in (0, 1)$.

So condition says that $f(\boldsymbol{\theta}^{[k]} + \boldsymbol{\Delta}_\alpha) < f(\boldsymbol{\theta}^{[k]})$ by a margin.

Then there is a **curvature condition**:

$$\nabla f(\boldsymbol{\theta}^{[k]} + \boldsymbol{\Delta}_\alpha)^\mathsf{T} \boldsymbol{\Delta}_\alpha \geq c_2 \nabla f(\boldsymbol{\theta}^{[k]})^\mathsf{T} \boldsymbol{\Delta}_\alpha,$$

with $c_2 \in (c_1, 1)$.

Substracting $\nabla f(\boldsymbol{\theta}^{[k]})^\mathsf{T} \boldsymbol{\Delta}_\alpha$ from both sides

$$(\nabla f(\boldsymbol{\theta}^{[k]} + \boldsymbol{\Delta}_\alpha) - \nabla f(\boldsymbol{\theta}^{[k]}))^\mathsf{T} \boldsymbol{\Delta}_\alpha \geq (c_2 - 1) \nabla f(\boldsymbol{\theta}^{[k]})^\mathsf{T} \boldsymbol{\Delta}_\alpha,$$

or

$$\rho_k^{-1} \geq (c_2 - 1) \nabla f(\boldsymbol{\theta}^{[k]})^\mathsf{T} \boldsymbol{\Delta}_\alpha > 0.$$

So it guarantees that $\mathbf{B}^{[k+1]}$ will be pos def.

Relative to Newton's method, with BFGS:

- You do not need to find the Hessian;
- You do not need to solve $\boldsymbol{\Delta}_\alpha = \mathbf{H}^{-1}\nabla f$ which is $O(p^3)$;
- Step will not be as good as Newton because you are approximating $\mathbf{H}$;
- You need to initialise $\mathbf{B}^{[0]}$.

Let's look at some examples:

```r
library(FLtools)
FLtools::optimisation()
```

What if I don't want to compute $\nabla f(\boldsymbol{\theta})$?

You can try the **Nelder-Mead** or **downhill symplex** optimiser.

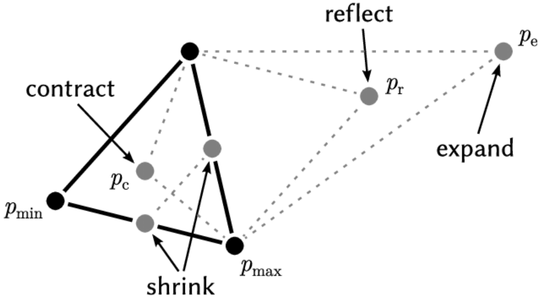


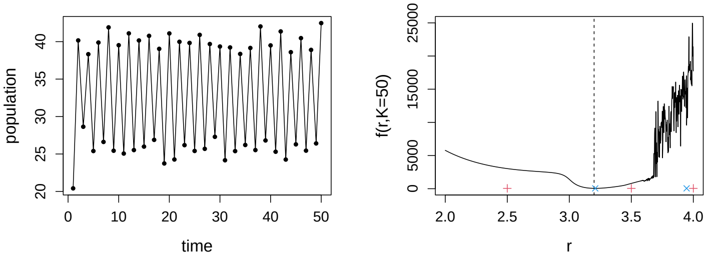
Figure 1: From Wikipedia

NOTE: it's the default optimiser in `stats::optim()`.

For examples, see `FLtools::optimisation()`.

Leading to the next part

We mentioned that it's important to look at your objective.

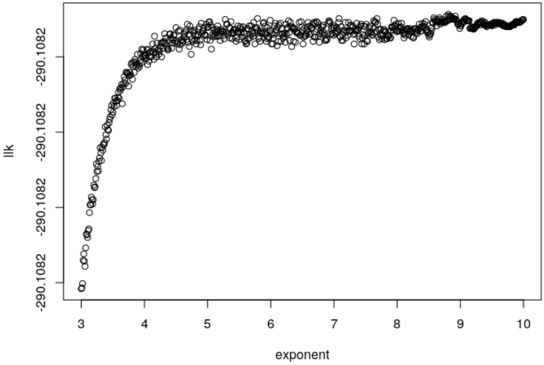


But in which direction should we look when $D \gg 1$?

SD, Newton and BGFS provide a search direction $\boldsymbol{\Delta}$.

That's the first direction along which to look.

Here is a real-world example I've encountered.



- y-axis is loglik($\boldsymbol{\theta} + \alpha \boldsymbol{\Delta}$)
- x-axis is γ used in

$$\alpha = \frac{1}{2^{\gamma}}$$

Objective is deterministic but evaluated up to **numerical noise**.