NTNU | Norwegian University of Science and Technology

TTK4135 – Lecture 13
Unconstrained optimization

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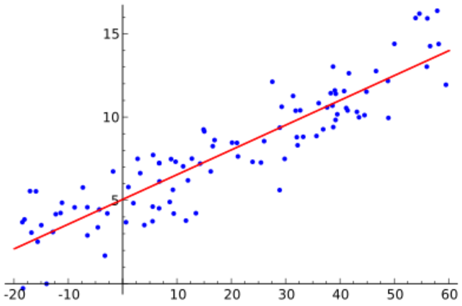
Outline

- Optimality conditions for unconstrained optimization
- Ingredients in gradient descent algorithms for unconstrained optimization
  - Descent directions (steepest descent, Newton, Quasi-Newton)
  - How far to walk in descent direction (line search, trust region)
  - Termination criteria
- Scaling

Reference: N&W Ch.2.1-2.2

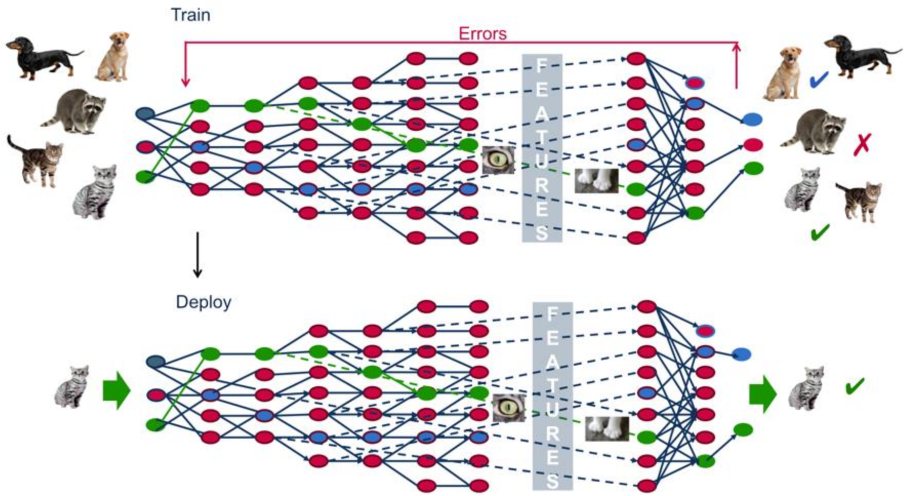
Example: Machine Learning

- Learn, and make predictions, from data



Wikipedia.org

- Linear regression is the most basic ML algorithm, solved using optimization
  - Linear least squares: Explicit solution
  - Nonlinear least squares: Ch. 10, N&W



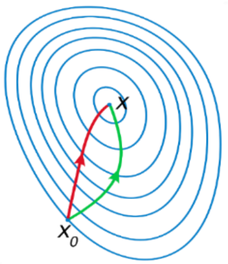
- In a similar fashion: ML, neural networks, deep learning etc. are “trained” using gradient descent algorithms
  - Gradient descent for unconstrained optimization is topic of Ch. 2-10, N&W

Learning goal Ch. 2, 3 and 6: Understand this slide

Line-search unconstrained optimization

$$\min_x f(x)$$

1. Initial guess x_0
2. While termination criteria not fulfilled
   a) Find descent direction p_k from x_k
   b) Find appropriate step length α_k ; set $x_{k+1} = x_k + \alpha_k p_k$
   c) $k = k+1$
3. $x_M = x^*$? (possibly check sufficient conditions for optimality)



A comparison of steepest descent and Newton's method. Newton's method uses curvature information to take a more direct route. (wikipedia.org)

Termination criteria:
Stop when first of these become true:

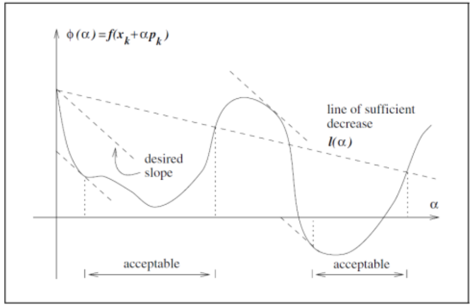
- $\|\nabla f(x_k)\| \leq \epsilon$ (necessary condition)
- $\|x_k - x_{k-1}\| \leq \epsilon$ (no progress)
- $\|f(x_k) - f(x_{k-1})\| \leq \epsilon$ (no progress)
- $k \leq k_{\max}$ (kept on too long)

Descent directions:

- Steepest descent
  $p_k = -\nabla f(x_k)$
- Newton
  $p_k = -(\nabla^2 f(x_k))^{-1} \nabla f(x_k)$
- Quasi-Newton
  $p_k = -B_k^{-1} \nabla f(x_k)$
  $B_k \approx \nabla^2 f(x_k)$

How to calculate derivatives – Ch. 8

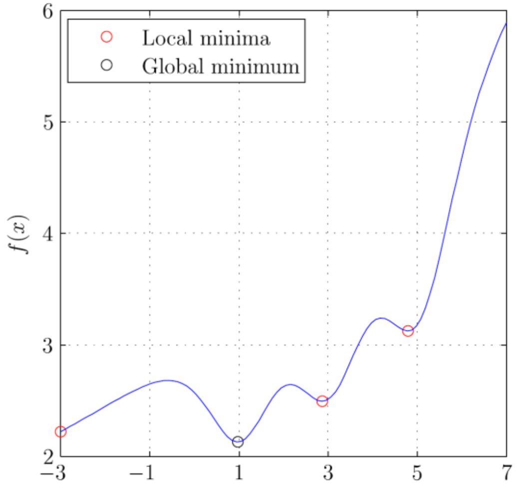
Step length line search (Wolfe):

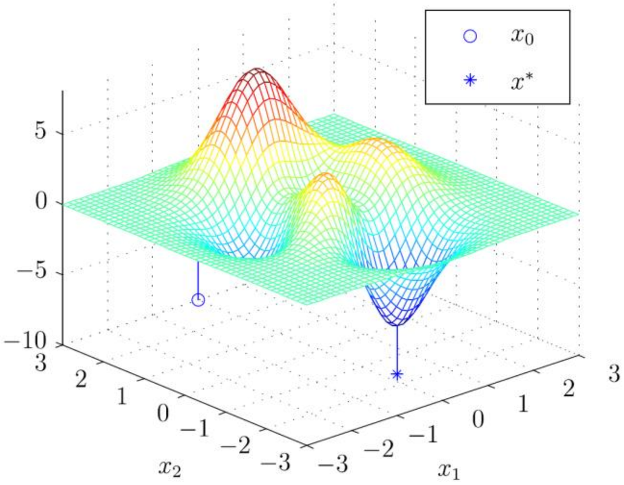


How many iterations? (Convergence rates)

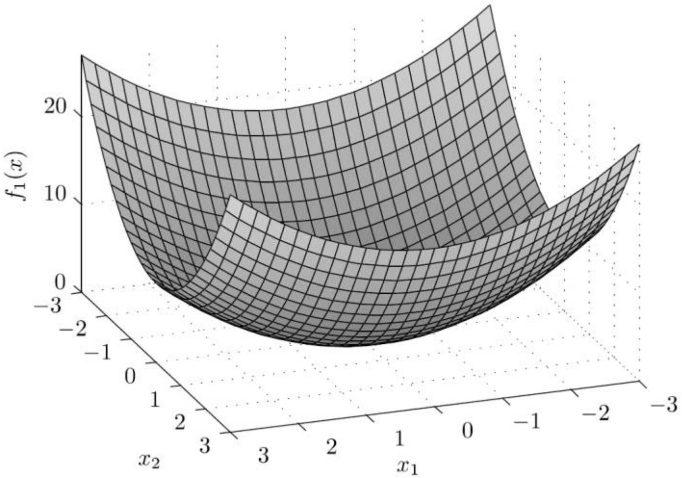
Unconstrained optimization

What is a solution? Local and global minimizers

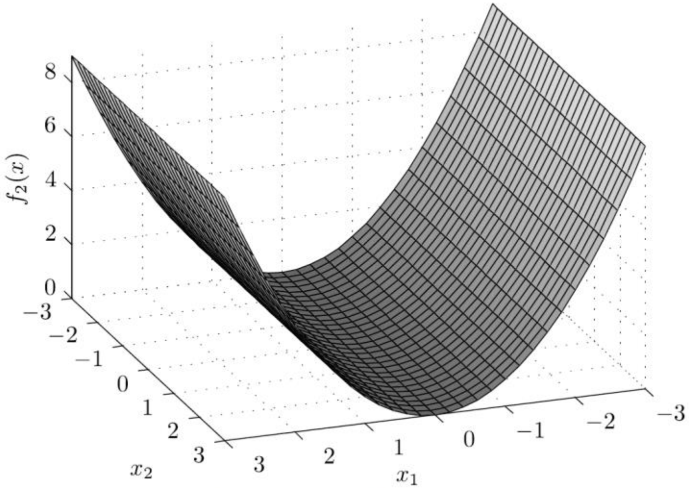




(Strict and non-strict optimizers)



$x^* = 0$ is a *strict minimizer.*



$x_1^* = 0$ is a *non-strict minimizer.*

Necessary condition for optimality

$$\min_x f(x)$$

Theorem 2.2: x^* local solution and $f \in C^1 \Rightarrow \nabla f(x^*) = 0$

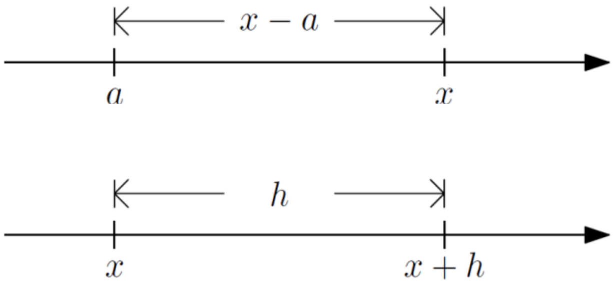
Taylor expansions

- From Calculus?

$$f(x) = f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2} f''(a) + \cdots$$

- In this course:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \cdots$$



Taylor's theorem

$$f : \mathbb{R}^n \to \mathbb{R},\ p \in \mathbb{R}^n$$

- First order: If *f* is continuously differentiable,

$$f(x+p) = f(x) + \nabla f(x+tp)^\top p, \quad \text{for some } t \in (0,1)$$

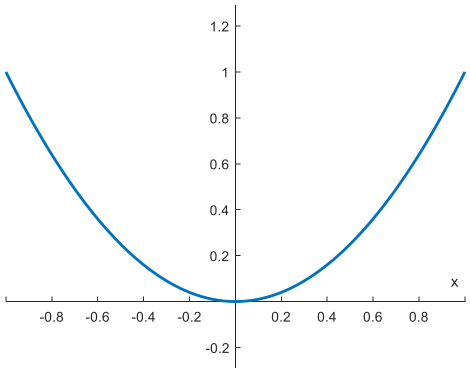
- Second order: If *f* is twice continuously differentiable

$$f(x+p) = f(x) + \nabla f(x)^\top p + \frac{1}{2} p^\top \nabla^2 f(x+tp)^\top p, \quad \text{for some } t \in (0,1)$$

Sufficient conditions for optimality

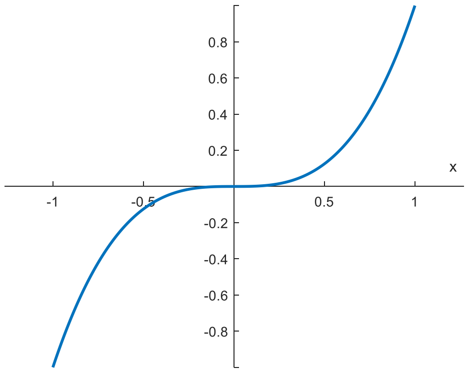
Theorem 2.4: $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*) > 0 \Rightarrow x^*$ strict local solution

x^2



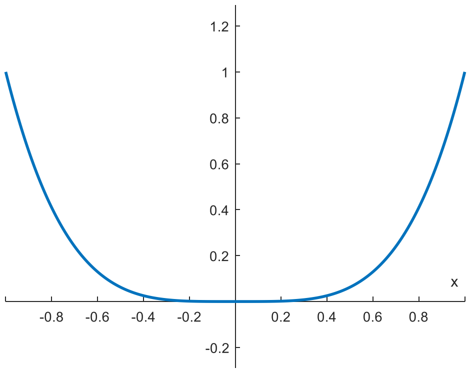
$$\nabla f(0) = 0$$
$$\nabla^2 f(0) > 0$$

x^3



$$\nabla f(0) = 0$$
$$\nabla^2 f(0) = 0$$

x^4

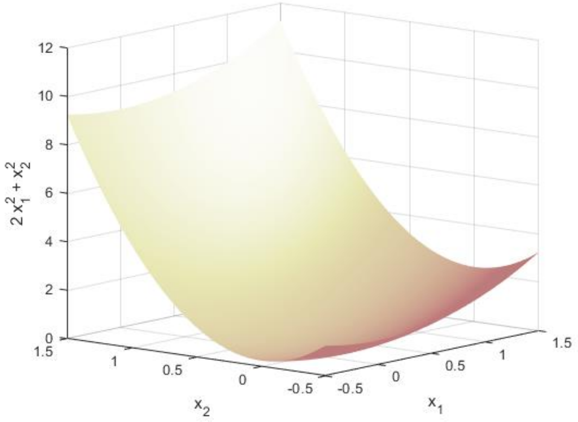


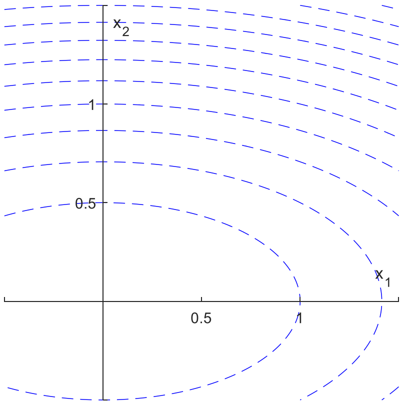
$$\nabla f(0) = 0$$
$$\nabla^2 f(0) = 0$$

General algorithm for solving $\min_x f(x)$

Termination criteria

Descent (downhill) directions





Quadratic approximation to objective function

$$f(x_k + p) \approx m_k(p) = f(x_k) + p^\top \nabla f(x_k) + \frac{1}{2} p^\top \nabla^2 f(x_k) p$$

Minimize approximation:

$$\nabla_p m_k(p) = 0 \Rightarrow p_k = -\left(\nabla^2 f(x_k)\right)^{-1} \nabla f(x_k)$$

“Newton step”:

$$x_{k+1} = x_k + p_k = x_k - \left(\nabla^2 f(x_k)\right)^{-1} \nabla f(x_k)$$

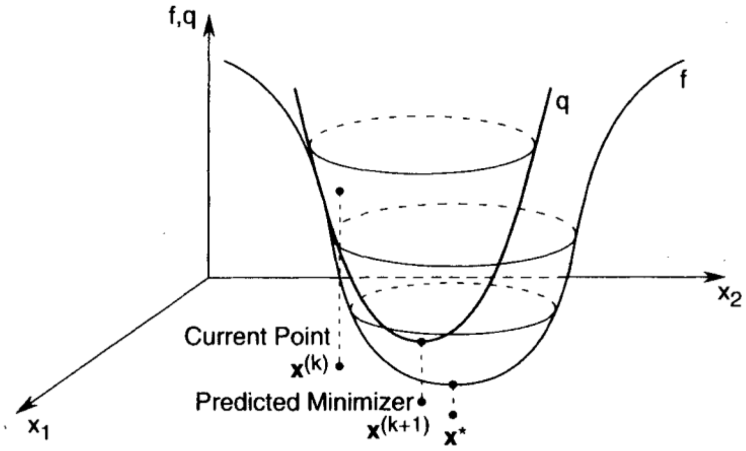
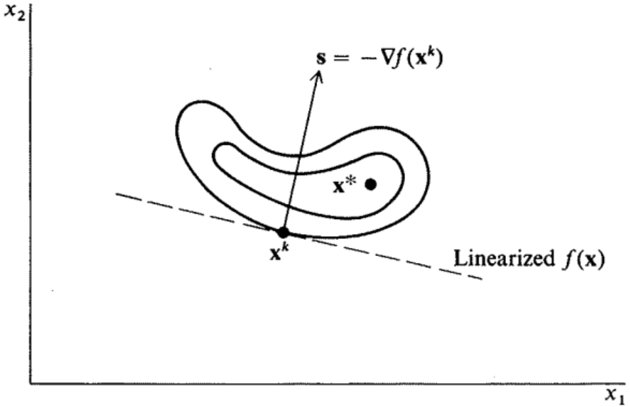


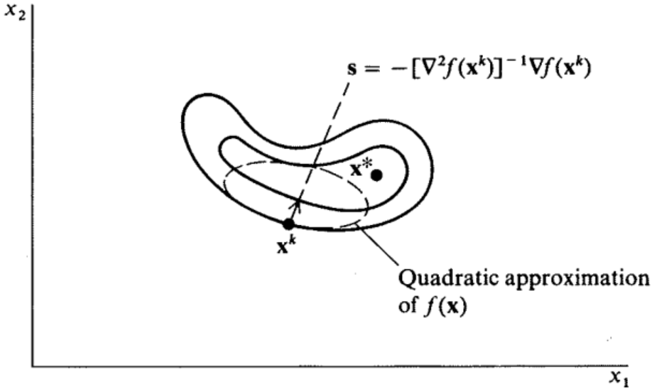
Figure 9.1 Quadratic approximation to the objective function using first and second derivatives.

Chong & Zak, “An introduction to optimization”

Steepest descent directions vs Newton directions from objective function approximations



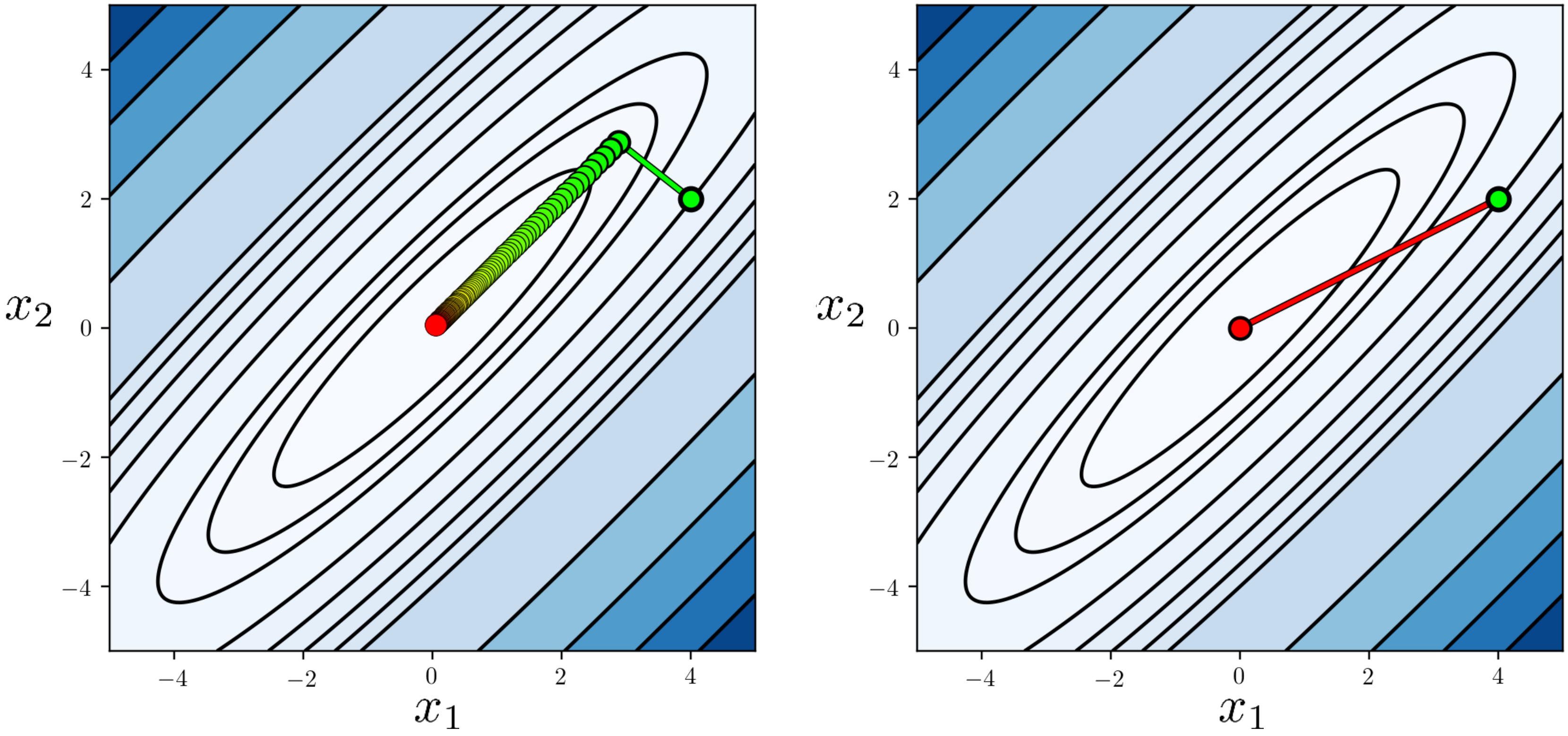
(a) Steepest descent: first-order approximation (linearization) of $f(\mathbf{x})$ at $\mathbf{x}^k$



(b) Newton's method: second-order (quadratic) approximation of $f(\mathbf{x})$ at $\mathbf{x}^k$

From Edgar, Himmelblau, Lasdon: “Optimization of Chemical Processes”

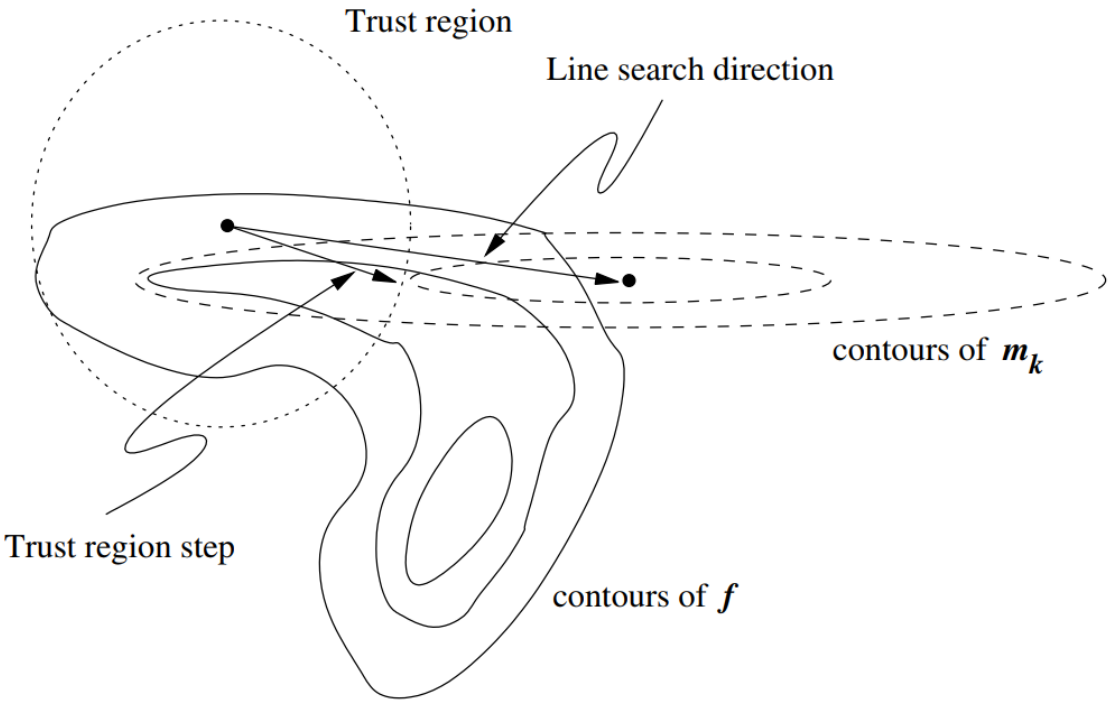
Steepest descent vs Newton



https://jermwatt.github.io/

How far should we walk along p_k?

Newton line search and trust region steps



Scaling, scale invariance

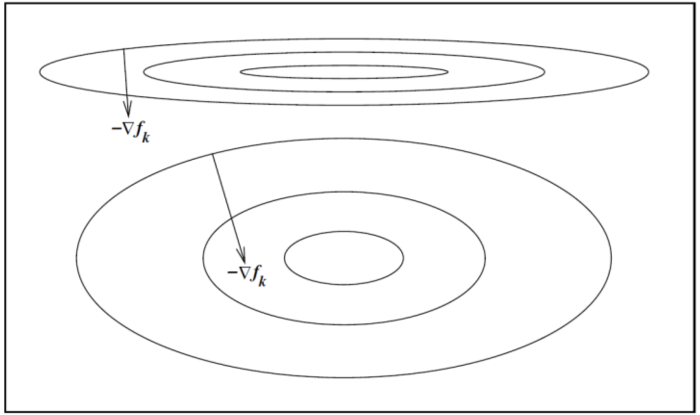


Figure 2.7 Poorly scaled and well scaled problems, and performance of the steepest descent direction.