Pattern Recognition (PR)

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This is a printable version of the slides of the lecture

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Prof. Dr.-Ing. Andreas Maier

Optimization

Motivation

- Optimization is crucial for many solutions in pattern recognition, pattern analysis, machine learning, artificial intelligence, etc.
- Optimization has many faces:
  - discrete optimization,
  - combinatorial optimization,
  - genetic algorithms,
  - gradient descent,
  - unconstrained and constrained optimization,
  - linear programming,
  - convex optimization, etc.
- There is no lecture on pattern recognition without a refresher course on optimization techniques.
- Each researcher has his own favorite optimization algorithm.

Convexity

Definition

A function $f : \mathbb{R}^d \to \mathbb{R}$ is *convex* if the domain $\text{dom}(f)$ of f is a convex set and if $\forall \boldsymbol{x}, \boldsymbol{y} \in \text{dom}(f)$, and θ with $0 \leq \theta \leq 1$, we have

$$f(\theta \boldsymbol{x} + (1-\theta)\boldsymbol{y}) \leq \theta f(\boldsymbol{x}) + (1-\theta) f(\boldsymbol{y})$$

A function $f : \mathbb{R}^d \to \mathbb{R}$ is *concave* if $-f$ is convex.

Geometric interpretation:

The line segment between $(\boldsymbol{x}, f(\boldsymbol{x}))$ and $(\boldsymbol{y}, f(\boldsymbol{y}))$ lies above the graph of f.

Unconstrained Optimization

Let us assume in the following that we have to compute the minimum of a convex function

$$f : \mathbb{R}^d \to \mathbb{R}$$

that is twice differentiable.

The unconstrained optimization problem is just the solution of the minimization problem

$$\boldsymbol{x}^* = \underset{\boldsymbol{x}}{\text{argmin}}\, f(\boldsymbol{x})$$

where $\boldsymbol{x}^*$ denotes the optimal point.

Unconstrained Optimization (cont.)

For this particular family of functions, a necessary and sufficient condition for the minumum are the zero-crossings of the function's gradient:

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

Unconstrained Optimization (cont.)

Most methods follow an iterative scheme:

$$\begin{array}{rl} \text{initialization} & \boldsymbol{x}^{(0)} \\ \text{iteration step} & \boldsymbol{x}^{(k+1)} = g(\boldsymbol{x}^{(k)}) \end{array}$$

where $g : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is the update function.

The iterations terminate, if

$$\|\boldsymbol{x}^{(k+1)} - \boldsymbol{x}^{(k)}\| < \varepsilon,$$

i. e. no further significant change.

Descent Methods

We now consider iteration schemes that produce a sequence of estimates according to the update function

$$\boldsymbol{x}^{(k+1)} = g(\boldsymbol{x}^{(k)}) = \boldsymbol{x}^{(k)} + t^{(k)} \Delta \boldsymbol{x}^{(k)}.$$

where

$\Delta \boldsymbol{x}^{(k)} \in \mathbb{R}^d$:	is the search direction in the k-th iteration
$t^{(k)} \in \mathbb{R}$:	denotes the step length in the k-th iteration

and where we expect

$$f(\boldsymbol{x}^{(k+1)}) < f(\boldsymbol{x}^{(k)}), \quad \text{i.e.} \ \nabla f(\boldsymbol{x}^{(k)})^T \Delta \boldsymbol{x}^{(k)} < 0$$

except $\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} = \boldsymbol{x}^*$.

Taylor Approximation

For many problems it is always good to know the second order Taylor approximation:

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

Descent Methods (cont.)

Input: function f, initial estimate $\boldsymbol{x}^{(0)}$
Initialize: $k := 0$
repeat
Select (or compute) descent direction
Line search (1-D optimization):

$$t^{(k)} = \underset{t \geq 0}{\operatorname{argmin}} f(\boldsymbol{x}^{(k)} + t \cdot \Delta \boldsymbol{x}^{(k)})$$

Update:

$$\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} + t^{(k)} \Delta \boldsymbol{x}^{(k)}.$$

$k := k + 1$
until $\|\boldsymbol{x}^{(k)} - \boldsymbol{x}^{(k-1)}\| < \varepsilon$
Output: $\boldsymbol{x}^{(k)}$

Line Search Methods

- Multivariate optimization in its described form requires a proper line search method.
- Exact line search along the straight line $\{\boldsymbol{x} + t\Delta\boldsymbol{x} \mid t \geq 0\}$ has to solve

$$t^* = \underset{t \geq 0}{\operatorname{argmin}} f(\boldsymbol{x} + t\Delta\boldsymbol{x})$$

  and is rarely used.
- An overview of methods can be found in numerical recipes.

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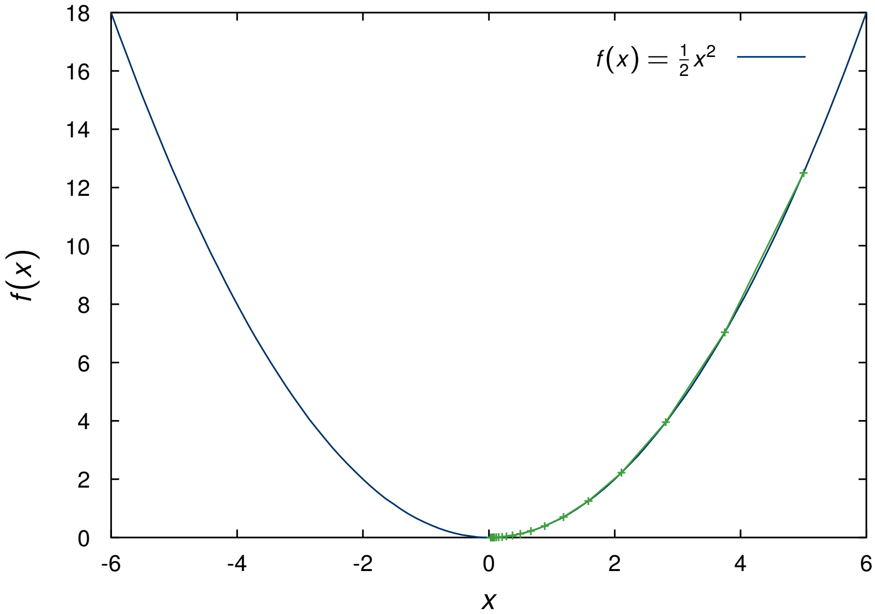
Line Search Methods (cont.)

Setting $t = 0.25$:



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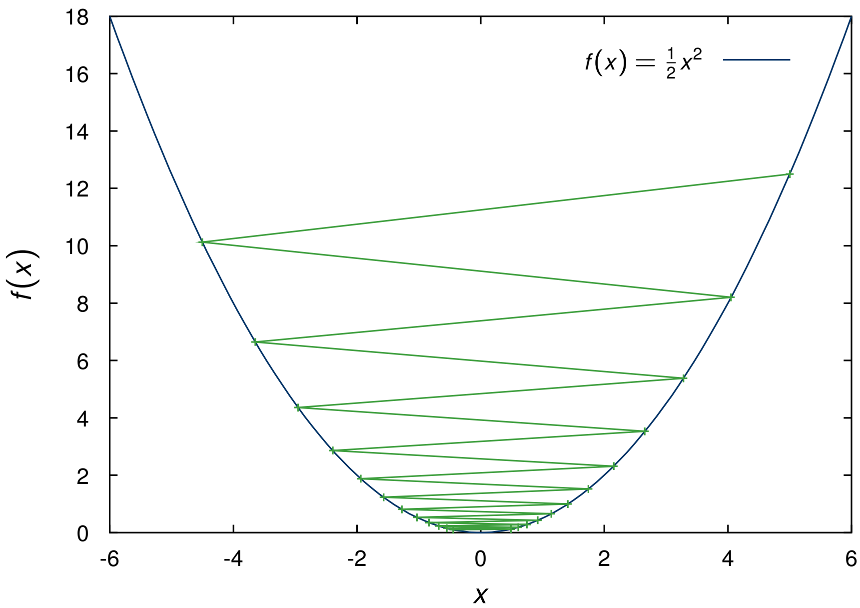
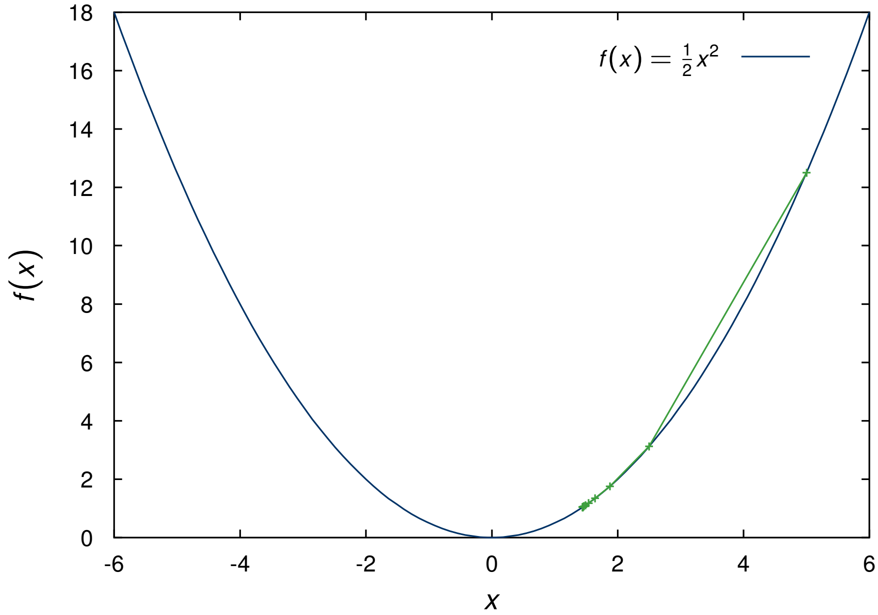
Line Search Methods (cont.)

Setting $t = 1.9$:



Line Search Methods (cont.)

Setting $t^{(k+1)} = \frac{1}{2} t^{(k)}$ and starting with $t^{(0)} = 0.5$:



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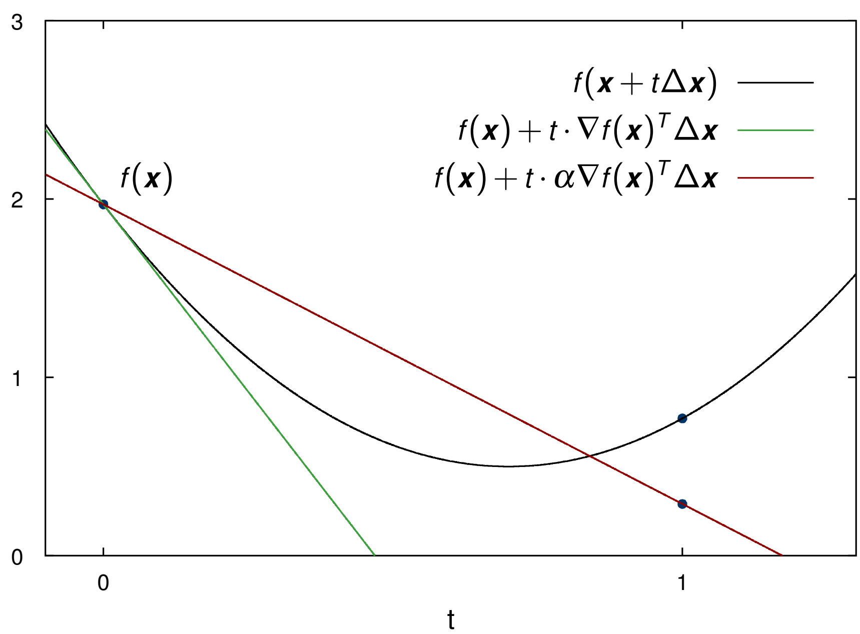
Backtracking Line Search



Backtracking Line Search (cont.)

The Armijo-Goldstein line search algorithm:

Input: function f, search direction $\Delta \boldsymbol{x}$
Initialize: $t := 1$
Select: $\alpha \in [0, 0.5]$ and $\beta \in [0, 1]$.
while $f(\boldsymbol{x} + t\Delta\boldsymbol{x}) > f(\boldsymbol{x}) + \alpha t \cdot \nabla f(\boldsymbol{x})^T \Delta \boldsymbol{x}$ **do**
  $t := \beta t$
end while
Output: t

Gradient Descent Methods

A natural choice of the search direction is the negative gradient:

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

Rule of thumb:

The negative gradient is the steepest descent direction.

Gradient Descent Methods (cont.)

Input: function f, initial estimate $\boldsymbol{x}^{(0)}$
intialize: $k := 0$
repeat
Set descent direction: $\Delta \boldsymbol{x}^{(k)} = -\nabla f(\boldsymbol{x}^{(k)})$
Line search (1-D optimization):

$$t^{(k)} = \operatorname*{argmin}_{t \geq 0} f(\boldsymbol{x}^{(k)} + t \cdot \Delta \boldsymbol{x}^{(k)})$$

Update:

$$\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} + t^{(k)} \Delta \boldsymbol{x}^{(k)}.$$

$k := k + 1$
until $\|\boldsymbol{x}^{(k)} - \boldsymbol{x}^{(k-1)}\|_2 < \varepsilon$
Output: $\boldsymbol{x}^{(k)}$

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Steepest Descent Methods

(Normalized) steepest descent, what does it mean?

We search for the unit vector that shows the largest decrease in the linear approximation of f:

$$\Delta \boldsymbol{x} = \underset{\boldsymbol{u}}{\operatorname{argmin}} \{\nabla f(\boldsymbol{x})^T \boldsymbol{u};\ \|\boldsymbol{u}\|_p = 1\}$$

Conclusions:

- The steepest descent direction depends on the chosen norm.
- The negative gradient is not necessarily the best choice for the search direction.

Steepest Descent Methods (cont.)

We consider now the first order Taylor approximation of $f(\boldsymbol{x} + \boldsymbol{u})$ around the selected position $\boldsymbol{x}$:

$$f(\boldsymbol{x} + \boldsymbol{u}) \approx f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^T \boldsymbol{u}.$$

- Here $\nabla f(\boldsymbol{x})^T \boldsymbol{u}$ is the directional derivative at $\boldsymbol{x}$ in direction $\boldsymbol{u}$.
- The vector $\boldsymbol{u}$ denotes a descent direction if the inner product with the gradient vetor is negative, i. e.

$$\nabla f(\boldsymbol{x})^T \boldsymbol{u} < 0\ .$$

Steepest Descent Methods (cont.)

Input: function f, initial estimate $\boldsymbol{x}^{(0)}$, norm $\|.\|$
intialize: $k := 0$
repeat

Compute highest descent direction:

$$\Delta \boldsymbol{x}^{(k)} = \underset{\boldsymbol{u}}{\operatorname{argmin}} \{ \nabla f(\boldsymbol{x}^{(k)})^T \boldsymbol{u};\ \|\boldsymbol{u}\| = 1 \}$$

Line search (1-D optimization):

$$t^{(k)} = \underset{t \geq 0}{\operatorname{argmin}}\, f(\boldsymbol{x}^{(k)} + t \cdot \Delta \boldsymbol{x}^{(k)})$$

Update:

$$\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} + t^{(k)} \Delta \boldsymbol{x}^{(k)}.$$

$k := k + 1$
until $\|\boldsymbol{x}^{(k)} - \boldsymbol{x}^{(k-1)}\| < \varepsilon$
Output: $\boldsymbol{x}^{(k)}$

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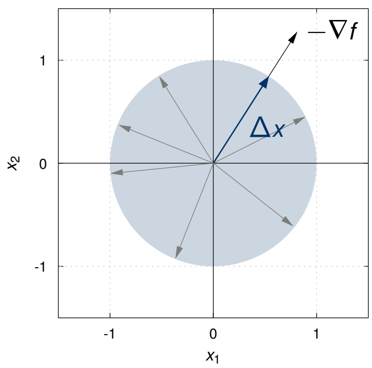
L_2-Norm

The unit ball for the L_2-norm:

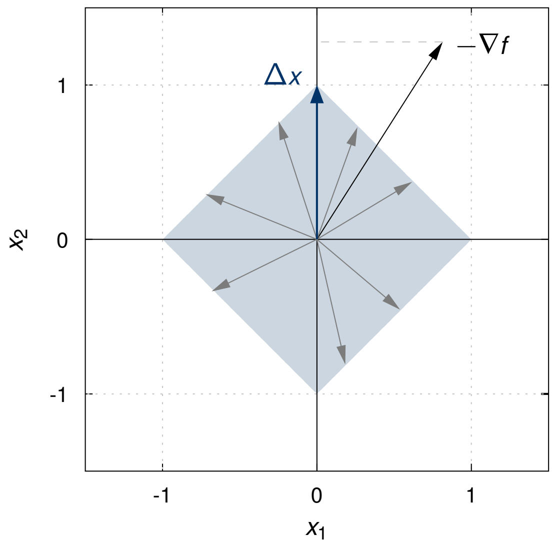


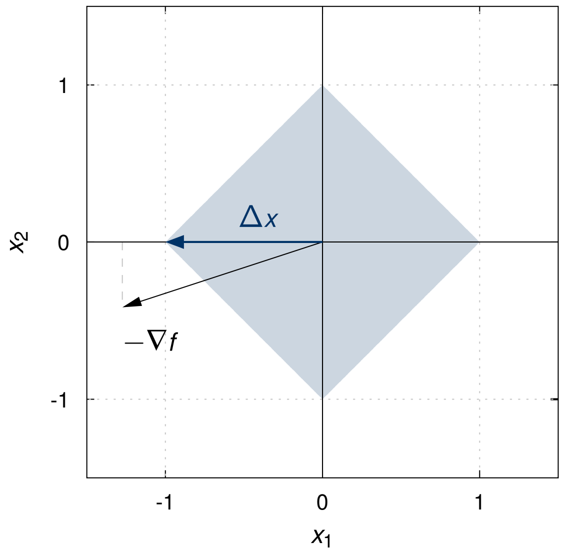
For the L_2-norm the steepest descent direction is the negative gradient:

$$\Delta \boldsymbol{x} = \underset{\boldsymbol{u}}{\operatorname{argmin}} \{ \nabla f(\boldsymbol{x})^T \boldsymbol{u};\ \|\boldsymbol{u}\|_2 = 1 \} = -\nabla f(\boldsymbol{x})$$

L_1-Norm

The unit ball for the L_1-norm:





L_1-Norm (cont.)

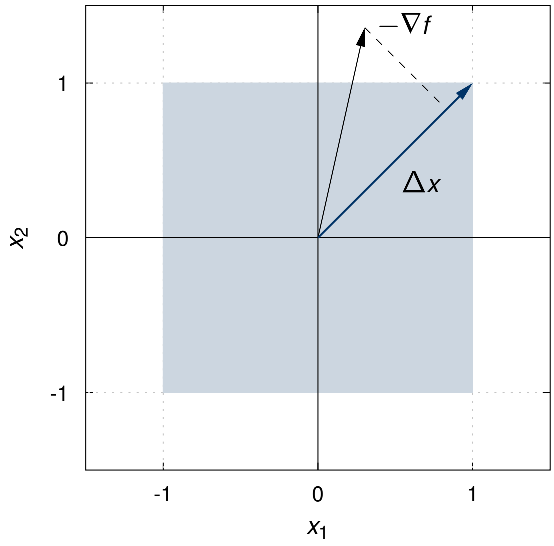
- The steepest descent for the L_1-norm selects in each iteration the component of $\nabla f(\boldsymbol{x})$ with maximum absolute value and then decreases or increases dependent on the sign of the selected component.
- Let i be the index of the gradient component with maximum absolute value, and let $\boldsymbol{e}_i \in \mathbb{R}^d$ denote the corresponding base vector.
  The steepest descent direction is given by:

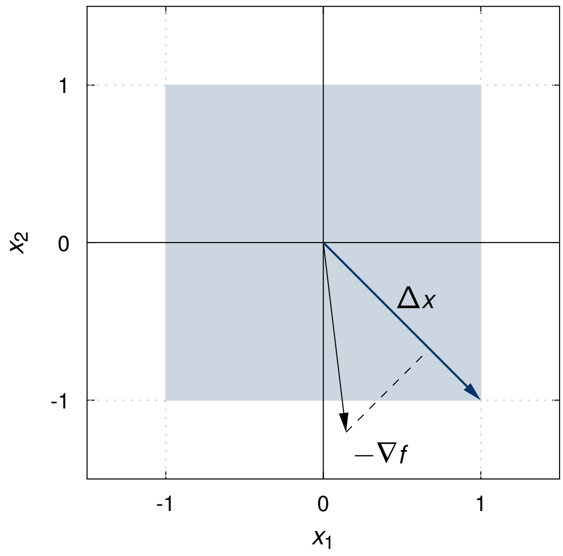
$$\begin{aligned}\Delta \boldsymbol{x} &= \operatorname*{argmin}_{\boldsymbol{u}} \{\nabla f(\boldsymbol{x})^T \boldsymbol{u};\ \|\boldsymbol{u}\|_1 = 1\} \\ &= -\operatorname{sgn}\left(\frac{\partial}{\partial x_i} f(\boldsymbol{x})\right) \boldsymbol{e}_i\end{aligned}$$

- Note: Steepest descent using the L_1-norm results in the *coordinate descent algorithm*.

L_∞-Norm

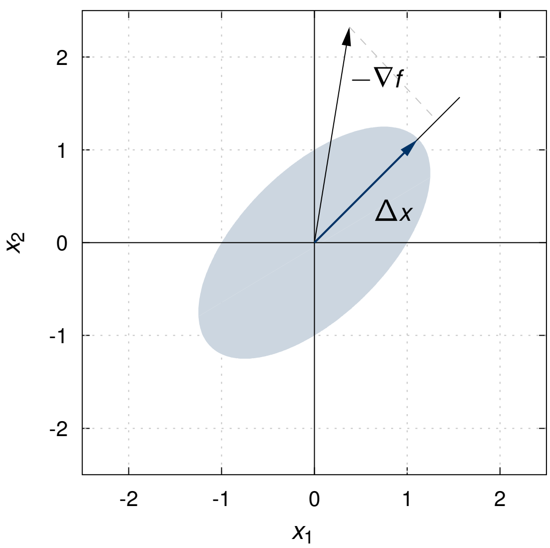
The unit ball for the L_∞-norm:





L_P-Norm

The unit ball for the L_P-norm:



L_P-Norm (cont.)

The steepest descent for the L_P-norm is given by:

$$\begin{aligned} \Delta \boldsymbol{x} &= \underset{\boldsymbol{u}}{\operatorname{argmin}} \{ \nabla f(\boldsymbol{x})^T \boldsymbol{u}; \ \|\boldsymbol{u}\|_{\boldsymbol{P}} = 1 \} \\ &= \underset{\boldsymbol{u}}{\operatorname{argmin}} \{ \nabla f(\boldsymbol{x})^T \boldsymbol{u}; \ (\boldsymbol{u}^T \boldsymbol{P} \boldsymbol{u})^{\frac{1}{2}} = 1 \} \\ &= \underset{\boldsymbol{u}}{\operatorname{argmin}} \{ \nabla f(\boldsymbol{x})^T \boldsymbol{u}; \ \|\boldsymbol{P}^{\frac{1}{2}} \boldsymbol{u}\|_2 = 1 \} \end{aligned}$$

As we did in the LDA-transform, we introduce a transform to get spherical data:

$$\boldsymbol{u}' = \boldsymbol{P}^{\frac{1}{2}} \boldsymbol{u}$$

and thus

$$f(\boldsymbol{u}) = f(\boldsymbol{P}^{-\frac{1}{2}} \boldsymbol{u}') = f'(\boldsymbol{u}')$$

L_P-Norm (cont.)

Instead of $f(\boldsymbol{x})$ we now minimize $f'(\boldsymbol{x}')$ using the L_2-norm and back-transform the result:

$$\begin{aligned} \Delta \boldsymbol{x}' &= \underset{\boldsymbol{u}}{\operatorname{argmin}} \{ \nabla f'(\boldsymbol{x}')^T \boldsymbol{u}'; \ \|\boldsymbol{u}'\|_2 = 1 \} \\ &= -\nabla f'(\boldsymbol{x}') \\ &= -\boldsymbol{P}^{-\frac{1}{2}} \nabla f(\boldsymbol{P}^{-\frac{1}{2}} \boldsymbol{x}') \\ &= -\boldsymbol{P}^{-\frac{1}{2}} \nabla f(\boldsymbol{x}) \end{aligned}$$

L_P-Norm (cont.)

Now we get for $\Delta \boldsymbol{x}$:

$$\begin{aligned}\Delta \boldsymbol{x} &= \boldsymbol{P}^{-\frac{1}{2}} \Delta \boldsymbol{x}' \\ &= \boldsymbol{P}^{-\frac{1}{2}} \left(-\boldsymbol{P}^{-\frac{1}{2}} \nabla f(\boldsymbol{x}) \right) \\ &= -\boldsymbol{P}^{-1} \nabla f(\boldsymbol{x}).\end{aligned}$$

Conclusion: The steepest descent for the L_P-norm is given by

$$\Delta \boldsymbol{x} = -\boldsymbol{P}^{-1} \nabla f(\boldsymbol{x}) \; .$$

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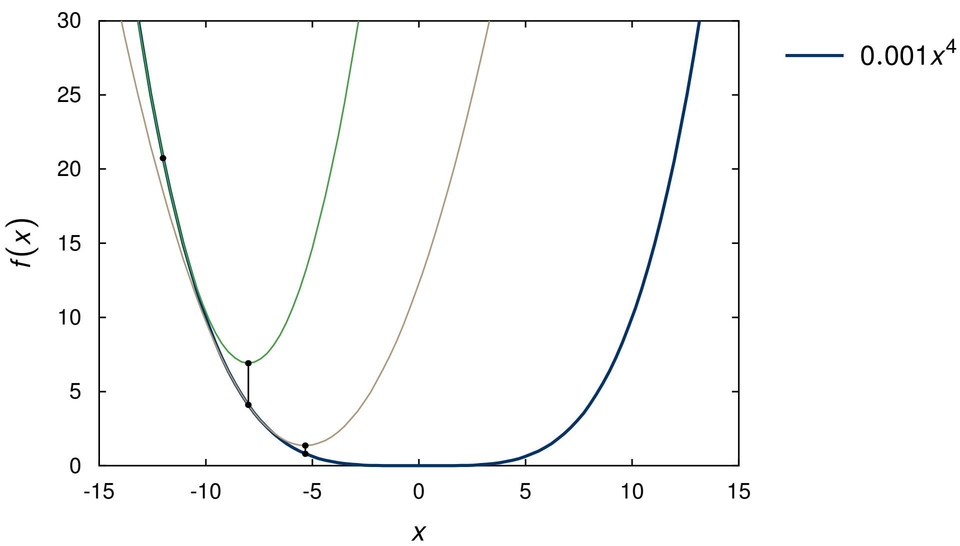
Newton's Method

The idea:

- Select a point.
- Compute the minimum of the second order Taylor approximation.



Newton's Method (cont.)

Second order Taylor approximation:

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

Now we select $\Delta\boldsymbol{x}$ such that

$$\nabla\{f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^T \Delta\boldsymbol{x} + \frac{1}{2}\Delta\boldsymbol{x}^T(\nabla^2 f(\boldsymbol{x}))\Delta\boldsymbol{x}\} = 0$$

Obviously the gradient is

$$\nabla f(\boldsymbol{x}) + \nabla^2 f(\boldsymbol{x})\Delta\boldsymbol{x} = 0$$

and thus

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

Newton's Method (cont.)

Conclusion:

Newton's method is an $\boldsymbol{x}$-dependent steepest descent method regarding the $L_{\boldsymbol{P}}$-norm, where $\boldsymbol{P} = \nabla^2 f(\boldsymbol{x})$ is the Hessian.

Damped Newton's Method

Input: function f, initial estimate $\boldsymbol{x}^{(0)}$
intialize: $k := 0$
repeat
Compute Newton step:

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

Line search (1-D optimization):

$$t^{(k)} = \operatorname*{argmin}_{t \geq 0} f(\boldsymbol{x}^{(k)} + t \cdot \Delta \boldsymbol{x}^{(k)})$$

Update:

$$\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} + t^{(k)} \Delta \boldsymbol{x}^{(k)}.$$

$k := k + 1$
until $\|\boldsymbol{x}^{(k)} - \boldsymbol{x}^{(k-1)}\| < \varepsilon$
Output: $\boldsymbol{x}^{(k)}$

Lessons Learned

- Gradient descent is widely applied.
- Gradient descent and coordinate descent are special cases of steepest descent methods.
- Steepest descent method depends on the chosen norm.

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Next Time in Pattern Recognition

  

Further Readings

This chapter is basically copied from:

- S. Boyd, L. Vandenberghe:
  Convex Optimization,
  Cambridge University Press, 2004.
  ☞ `http://www.stanford.edu/~boyd/cvxbook/`
- Jorge Nocedal, Stephen Wright:
  Numerical Optimization,
  Springer, New York, 1999.

Comprehensive Questions

- What is the general formulation for an unconstrained optimization problem?
- Why do we need a line search in gradient descent approaches?
- What is the Armijo-Goldstein line search algorithm?
- What are the steepest descent directions if we apply the L_∞, L_1, L_2, and $L_{\boldsymbol{P}}$ norm?