NTNU | Norwegian University of Science and Technology

TTK4135 – Lecture 16
Calculating derivatives and Derivative-free optimization

Lecturer: Lars Imsland

Lecture 16: Calculating derivatives (Ch. 8), and Derivative-free optimization (Ch. 9)

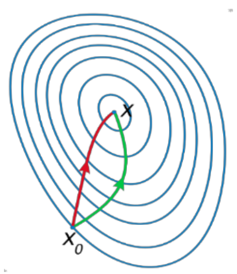
- Brief recap linesearch unconstrained optimization
- Calculating derivatives (gradient/Jacobian and Hessian)
- What can you do when obtaining derivatives is impractical?
  - Derivative-free optimization! For example: Nelder-Mead

Reference: N&W Ch. 8.1, (8.2), Ch. 9.1, 9.5

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:

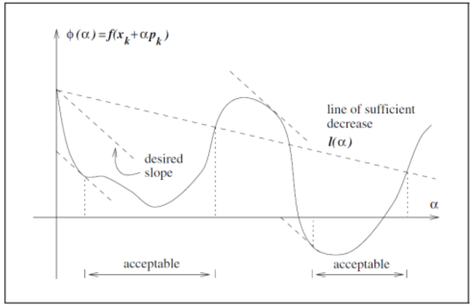
- $\|\nabla f(x_k)\| \leq \epsilon$ (necessary condition)
- $\|x_k - x_{k-1}\| \leq \epsilon$ (no progress)
- $\|f(x_k) - f(x_{k-1})\| \leq \epsilon$ (no progress)
- $k \leq k_{\max}$ (kept on too long)

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)

Quasi-Newton: BFGS method

$$p_k = -B_k^{-1}\nabla f(x_k)$$
$$B_k \approx \nabla^2 f(x_k)$$
$$H_k = B_k^{-1}$$

Algorithm 6.1 (BFGS Method).

Given starting point x_0, convergence tolerance $\epsilon > 0$,
  inverse Hessian approximation H_0;
$k \leftarrow 0$;
while $\|\nabla f_k\| > \epsilon$;
  Compute search direction

$$p_k = -H_k \nabla f_k;$$

  Set $x_{k+1} = x_k + \alpha_k p_k$ where α_k is computed from a line search procedure to satisfy the Wolfe conditions (3.6);
  Define $s_k = x_{k+1} - x_k$ and $y_k = \nabla f_{k+1} - \nabla f_k$;
  Compute H_{k+1} by means of (6.17);
  $k \leftarrow k + 1$;
end (while)

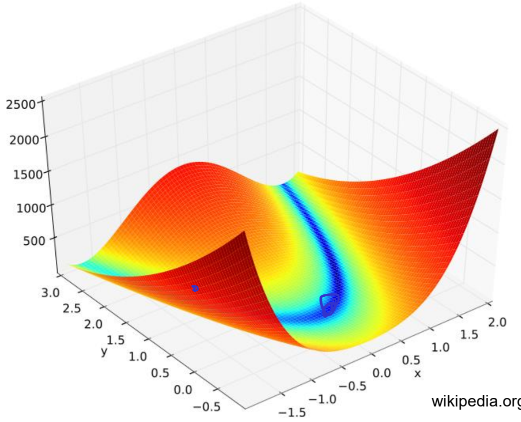
We use only gradient!

$$H_{k+1} = (I - \rho_k s_k y_k^T) H_k (I - \rho_k y_k s_k^T) + \rho_k s_k s_k^T$$

Example (from book)

- Using steepest descent, BFGS and inexact Newton on Rosenbrock function

$$f(x) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$



wikipedia.org

- Iterations from starting point (-1.2,1):
  - Steepest descent: 5264
  - BFGS: 34
  - Newton: 21

- Last iterations; value of $\|x_k - x^*\|$

steepest descent	BFGS	Newton
1.827e-04	1.70e-03	3.48e-02
1.826e-04	1.17e-03	1.44e-02
1.824e-04	1.34e-04	1.82e-04
1.823e-04	1.01e-06	1.17e-08

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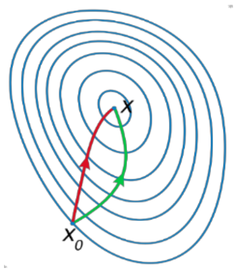

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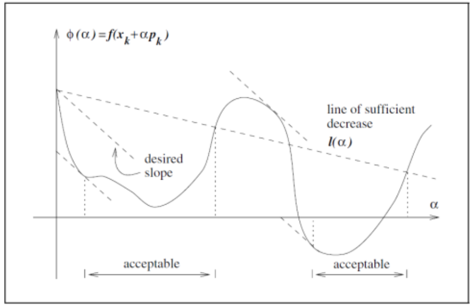
Step length line search (Wolfe):



Need derivatives! How to compute them?
And what if derivatives are not available, or too expensive to compute?

Four ways of finding derivatives

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- By hand
  - Time consuming and (very!) error prone for large problems

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  - Computer algebra systems (CAS)
    - GeoGebra, Maple, Mathematica, Matlab symbolic toolbox, pySym ...
    - Gives unreadable code, expensive to evaluate&compile, cumbersome to maintain

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  - Easy to implement (do it yourself), but may have low accuracy

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- **Numerical differentiation (finite differences)**
  - Easy to implement (do it yourself), but may have low accuracy

- **Automatic (Algorithmic) Differentiation (AD)**
  - Best option when it can be done
  - Easy to implement using the right software
  - Exact up to machine precision

Numerical differentiation

$f : \mathbb{R} \to \mathbb{R}$: $\quad \dfrac{df}{dx} = \dfrac{f(x+\varepsilon) - f(x)}{\varepsilon}$, ε "small number"

$f : \mathbb{R}^n \to \mathbb{R}$: directional derivative

$$\frac{d}{d\alpha} f(x+\alpha p) \Big|_{\alpha=0} = \nabla f(x)^T p \approx \frac{f(x+\varepsilon p) - f(x)}{\varepsilon}$$

$$\frac{\partial f}{\partial x_i} \approx \frac{f(x+\varepsilon e_i) - f(x)}{\varepsilon}$$

$$e_i = (0, \dots, 0, \overset{i}{1}, 0, \dots, 0)^T$$

Full gradient : Loop over $e_1, e_2, \dots, e_n$:

Theoretical accuracy of numerical differentiation

$f : \mathbb{R}^n \to \mathbb{R}$, assume $\|\nabla^2 f(x)\| \leq L$, $\forall x$

Taylor: $\left| f(x+p) - \left(f(x) + \nabla f(x)^T p \right) \right| = \frac{1}{2} \left| p^T \nabla^2 f(x+tp)\, p \right|$

$$\leq \frac{1}{2} \|\nabla^2 f(x+tp)\| \, \|p\|^2$$

$$\leq \frac{L}{2} \|p\|^2$$

Let $p = \varepsilon e_i$:

$$\Big| f(x+\varepsilon e_i) - f(x) - \varepsilon \underbrace{\nabla f(x)^T e_i}_{= \frac{\partial f}{\partial x_i}} \Big| \leq \frac{L}{2} \varepsilon^2$$

$$\left| \frac{f(x+\varepsilon e_i) - f(x)}{\varepsilon} - \frac{\partial f}{\partial x_i} \right| \leq \frac{L}{2} \varepsilon \quad \Rightarrow \quad \boxed{\frac{\partial f}{\partial x_i} = \frac{f(x+\varepsilon e_i) - f(x)}{\varepsilon} + O(\varepsilon)}$$

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

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

Finite differences and accuracy

One-sided difference: $$\frac{\partial f}{\partial x_i} = \frac{f(x+\epsilon e_i) - f(x)}{\epsilon} + O(\epsilon)$$

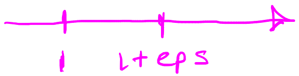
Two-sided difference: $$\frac{\partial f}{\partial x_i} = \frac{f(x+\epsilon e_i) - f(x-\epsilon e_i)}{2\epsilon} + O(\epsilon^2)$$

Theoretically: smaller ε $\rightarrow$ higher accuracy

However: Too small ε: Accuracy destroyed due to finite precision

"Optimal" trade-off (rule-of-thumb):

$\varepsilon = \sqrt{eps}$, eps "relative accuracy"



IEEE double:

$eps = 2^{-52} \approx 2 \cdot 10^{-16} \Rightarrow \varepsilon = 10^{-8}$

Commonly: ε between $10^{-6} - 10^{-8}$

```
>> eps
ans =
  2.2204e-16
```

Numerical differentiation (finite differences)

- Scalar $f : \mathbb{R} \to \mathbb{R}$: For some small ϵ,

$$\frac{\mathrm{d}f}{\mathrm{d}x} \approx \frac{f(x+\epsilon) - f(x)}{\epsilon}$$

- Directional derivative of $f : \mathbb{R}^n \to \mathbb{R}$

$$\nabla f^{\mathsf{T}} p \approx \frac{f(x+\epsilon p) - f(x)}{\epsilon}$$

- Full gradient ∇f: Directional derivatives along all axes $p = \epsilon e_i$
($e_1 = (1, 0, 0, \ldots)^{\mathsf{T}}, e_2 = (0, 1, 0, \ldots)^{\mathsf{T}}, \ldots$)
  - Note: Not necessary to calculate full gradient if you only need directional derivative! (**Also valid for AD!**)

- How to choose epsilon?
  - Theoretical error proportional to ϵ, but too small ϵ gives numerical noise
  - Rule of thumb: $\epsilon = \sqrt{\mathrm{eps}}$, where eps is machine precision (or precision of computing *f*) (IEEE double precision: $\epsilon = 10^{-8}$)

Approximating the Hessian

- In many cases, the gradient is available, but not the Hessian. We can then use finite differences on the gradient:

$$\nabla^2 f(x)p \approx \frac{\nabla f(x + \epsilon p) - \nabla f(x)}{\epsilon}$$

- If the gradient is not available, use finite differences “twice” for Hessian:

$$\frac{\partial^2 f}{\partial x_i \partial x_j}(x) = \frac{f(x + \epsilon e_i + \epsilon e_j) - f(x + \epsilon e_i) - f(x + \epsilon e_j) + f(x)}{\epsilon^2} + O(\epsilon)$$

(but usually better to use Quasi-Newton then…)

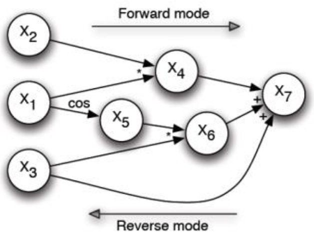
AD – Automatic (algorithmic) differentiation

- Software tools that automatically computes derivatives of your code
- The principle is simple: Extensive/automated use of ‘chain rule’

- Two modes; forward and reverse

- Two (main) implementation variants
  - Source code transformation
  - **Operator overloading** (object oriented language)

$$f(x_1, x_2, x_3) = x_1 x_2 + x_3 \cos(x_1) + x_3$$



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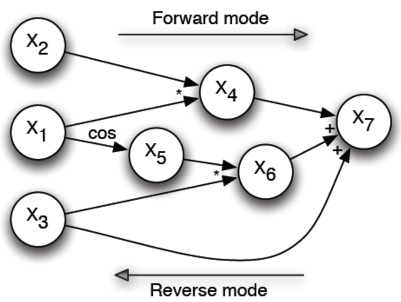
$x_7 = x_4 + x_6 + x_3$	$\frac{\partial x_7}{\partial x_3} = \frac{\partial x_7}{\partial x_4} = \frac{\partial x_7}{\partial x_6} = 1$

- Requires (more or less) that your implementation is differentiable
- Example software:
  - Optimization: ADOL-C, CppAD, CasADi, JuMP, …
  - Machine learning: Tensorflow, Pytorch, …

AD – forward and reverse

- Forward mode
  - Both x_i and ∇x_i are calculated by forward traversing computation graph

$$f(x_1, x_2, x_3) = x_1 x_2 + x_3 \cos(x_1) + x_3$$



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$$ABC$$
$$= (AB)C$$
$$= A(BC)$$

- Reverse mode
  - First, calculate x_i by traversing graph forward
  - Then, calculate derivatives by traversing graph backward

AD – forward vs. reverse

$$\nabla f = \begin{array}{cc} n & \\ \begin{bmatrix} & \vdots & \\ \cdots & \cdot & \cdots \\ & \vdots & \end{bmatrix} & m \end{array}$$

- Given a function $f : \mathbb{R}^n \to \mathbb{R}^m$
  - Costs of calculating derivatives with AD:
    - Forward mode (one "column"): $\text{cost}(\nabla f^\mathsf{T} p) \leq 2\ \text{cost}(f)$
    - Forward mode (entire Jacobian): $\text{cost}(\nabla f) \leq 2n\ \text{cost}(f)$
    - Reverse mode (one "row"): $\text{cost}(\lambda^\mathsf{T} \nabla f) \leq 3\ \text{cost}(f)$
    - Reverse mode (entire Jacobian): $\text{cost}(\nabla f) \leq 3m\ \text{cost}(f)$

AD – forward vs. reverse

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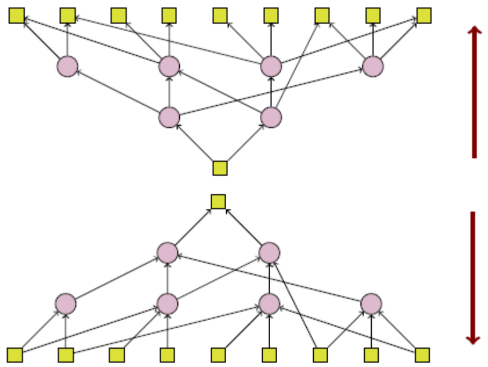
    - Reverse mode (entire Jacobian): $\text{cost}(\nabla f) \le 3m\ \text{cost}(f)$
  - Forward mode: Similar cost as numerical differentiation, but more accurate
  - If *m* >> *n*, forward mode is fastest
  - If *n* >> *m*, reverse mode is fastest



How AD software is implemented

- Prototype procedure:
  - Decompose original code into “intrinsic” functions (e.g. x_1x_2, sin(x), ln(x), etc.)
  - Differentiate the intrinsic functions (‘symbolically’, or make a lookup table) (sin(x)’ = cos(x), etc.)
  - Put everything together according to the chain rule (either forward or reverse mode)

- How to automatically transform your program into a program with derivatives? Two approaches:
  - Source code transformation (Typical: C, Fortran)
  - **Operator overloading** (C++, Fortran 90, Java, Matlab, Python, Julia, …)

Example (C/C++)

$$f(x_1, x_2, x_3) = x_1 x_2 + x_3 \cos(x_1) + x_3$$

function.c

```c
double f(double x1, double x2, double x3) {
   double x4, x5, x6, x7;

   x4 = x1*x2;
   x5 = cos(x1);
   x6 = x3*x5;
   x7 = x4 + x6 + x3;

   return x7;
}
```

function.c

Source code transformation (forward mode)

diff_function.c

```
double* f(double x1, double x2, double x3, double dx1, double dx2, double dx3) {
   double x4, x5, x6, x7, dx4, dx5, dx7, df[2];

   x4 = x1*x2;
   dx4 = dx1*x2 + x1*dx2;
   x5 = cos(x1);
   dx5 = -sin(x1)*dx1;
   x6 = x3*x5;
   dx6 = dx3*x5 + x3*dx5;
   x7 = x4 + x6 + x3;
   dx7 = dx4 + dx6 + dx3;

   df[0] = x7;
   df[1] = dx7;

   return df;
}
```

function.c → AD tool → **diff_function.c** → compiler → **diff_function.o**

Operator overloading example (using CppAD)

- Implement function as you do normally, but with other types (here: using C++ templates):

function.cpp

```
template <class vector>
vector f(vector x) {
   vector ... // possible temporary variables

   return x[1]*x[2] + x[3]*cos(x[1]) + x[3];
}
```

- Record operation sequence when you use the function:

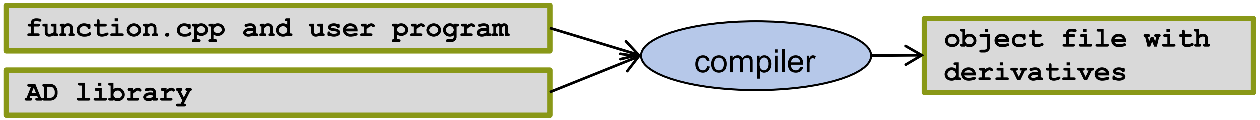
```
...
CppAD::vector<ADdouble> x(3), f_res;
x[1] = pi; x[2] = 4; x[3] = 3;

// declare that x contains the independent variables (and start recording)
CppAD::Independent(x);

f_res = f(x);

// create the AD function object F : x -> f_res (and stop recording)
CppAD::ADFun<double> F(x, f_res);

std::vector<double> jac( NS*NS ) = F.Jacobian;
...
```



Software etc.

- General information
  - http://www.autodiff.org/
  - http://en.wikipedia.org/wiki/Automatic_differentiation

- Many libraries of different maturity/robustness/performance, for different languages and for different applications

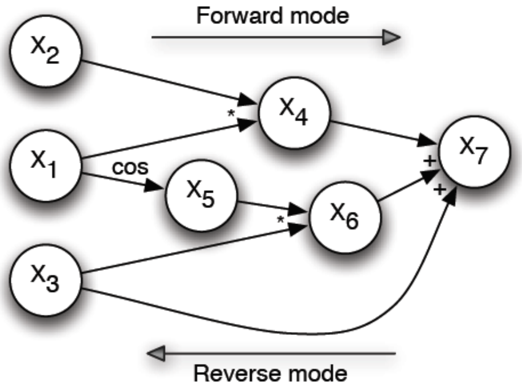
- Some mature libraries for optimization
  - C++: ADOL-C, CppAD
  - Developed for control&optimization: CasADi (Matlab/Octave, Python, C++)

- Book:
  - A. Griewank, **A. Walther**, “Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation”, 2nd edition. SIAM, 2008.

AD – example (from R. Ringset)

- Calculate gradient of $f(x_1, x_2, x_3) = x_1 x_2 + x_3 \cos(x_1) + x_3$

  at $[\ \pi \quad 4 \quad 3\ ]^T$



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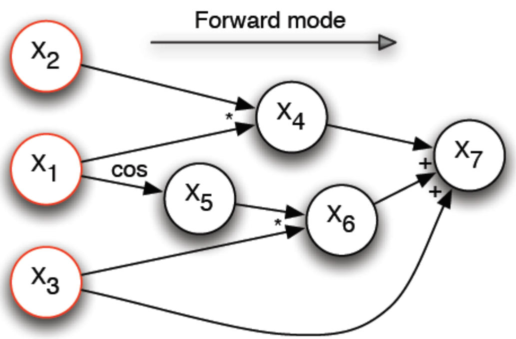
AD – forward mode

$$f(x_1, x_2, x_3) = x_1 x_2 + x_3 \cos(x_1) + x_3$$
$$x = (\pi, 4, 3)^\top$$

$$\nabla x_1 = e_1$$
$$\nabla x_2 = e_2$$
$$\nabla x_3 = e_3$$
$$\nabla x_4 = ?$$
$$\nabla x_5 = ?$$
$$\nabla x_6 = ?$$
$$\nabla x_7 = ?$$

$$e_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad e_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad e_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix};$$



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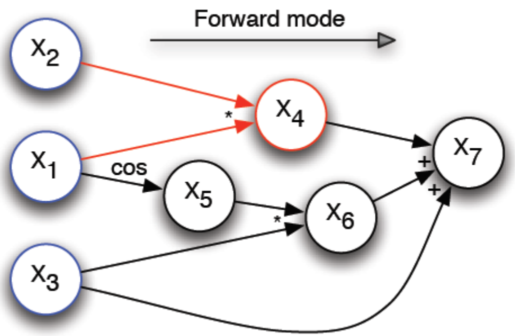
$$x = (\pi, 4, 3)^\top$$

$$\nabla x_1 = e_1$$
$$\nabla x_2 = e_2$$
$$\nabla x_3 = e_3$$
$$\nabla x_4 = \frac{\partial x_4}{\partial x_1} \nabla x_1 + \frac{\partial x_4}{\partial x_2} \nabla x_2 = \begin{bmatrix} x_2 & x_1 & 0 \end{bmatrix}^T = \begin{bmatrix} 4 & \pi & 0 \end{bmatrix}^T$$
$$\nabla x_5 = ?$$
$$\nabla x_6 = ?$$
$$\nabla x_7 = ?$$



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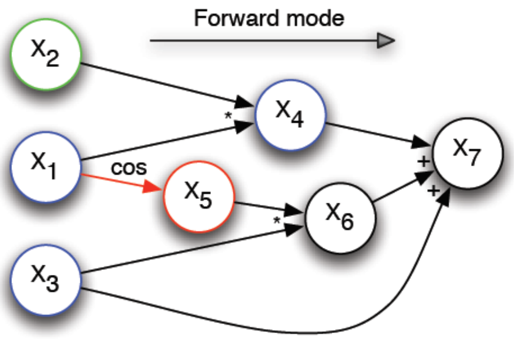
$$x = (\pi, 4, 3)^\top$$

$$\nabla x_1 = e_1$$
$$\nabla x_2 = e_2$$
$$\nabla x_3 = e_3$$
$$\nabla x_4 = \begin{bmatrix} 4 & \pi & 0 \end{bmatrix}^T$$
$$\nabla x_5 = \frac{\partial x_5}{\partial x_1} \nabla x_1 = -\sin(x_1) e_1 = 0$$
$$\nabla x_6 = ?$$
$$\nabla x_7 = ?$$

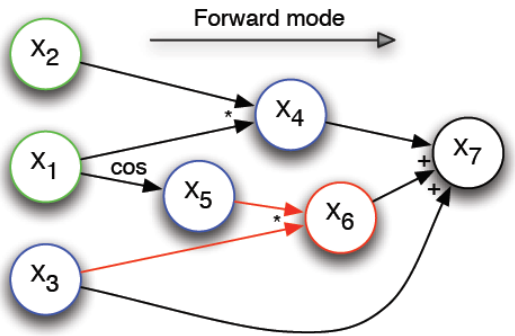


Variables	Derivatives
$x_4 = x_1 x_2$	$\frac{\partial x_4}{\partial x_1} = x_2, \frac{\partial x_4}{\partial x_2} = x_1$
$x_5 = \cos(x_1)$	$\frac{\partial x_5}{\partial x_1} = -\sin(x_1)$
$x_6 = x_5 x_3$	$\frac{\partial x_6}{\partial x_3} = x_5, \frac{\partial x_6}{\partial x_5} = x_3$
$x_7 = x_4 + x_6 + x_3$	$\frac{\partial x_7}{\partial x_3} = \frac{\partial x_7}{\partial x_4} = \frac{\partial x_7}{\partial x_6} = 1$

AD – forward mode

$$f(x_1, x_2, x_3) = x_1 x_2 + x_3 \cos(x_1) + x_3$$
$$x = (\pi, 4, 3)^\top$$

$$\nabla x_1 = e_1$$
$$\nabla x_2 = e_2$$
$$\nabla x_3 = e_3$$
$$\nabla x_4 = \begin{bmatrix} 4 & \pi & 0 \end{bmatrix}^T$$
$$\nabla x_5 = 0$$
$$\nabla x_6 = \frac{\partial x_6}{\partial x_3} \nabla x_3 + \frac{\partial x_6}{\partial x_5} \nabla x_5 = x_5 e_3 + x_3 0 = cos(\pi) e_3 = -e_3$$
$$\nabla x_7 = ?$$



Variables	Derivatives
$x_4 = x_1 x_2$	$\frac{\partial x_4}{\partial x_1} = x_2, \frac{\partial x_4}{\partial x_2} = x_1$
$x_5 = \cos(x_1)$	$\frac{\partial x_5}{\partial x_1} = -\sin(x_1)$
$x_6 = x_5 x_3$	$\frac{\partial x_6}{\partial x_3} = x_5, \frac{\partial x_6}{\partial x_5} = x_3$
$x_7 = x_4 + x_6 + x_3$	$\frac{\partial x_7}{\partial x_3} = \frac{\partial x_7}{\partial x_4} = \frac{\partial x_7}{\partial x_6} = 1$

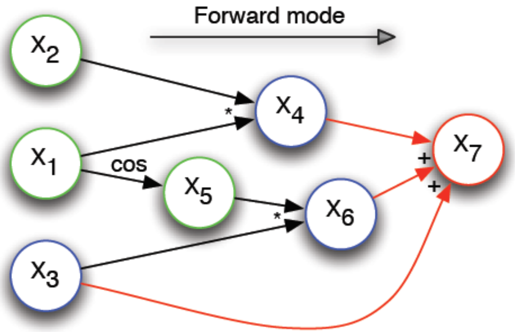
AD – forward mode

$$f(x_1, x_2, x_3) = x_1 x_2 + x_3 \cos(x_1) + x_3$$

$$x = (\pi, 4, 3)^\top$$

$$\nabla x_1 = e_1$$
$$\nabla x_2 = e_2$$
$$\nabla x_3 = e_3$$
$$\nabla x_4 = \begin{bmatrix} 4 & \pi & 0 \end{bmatrix}^T$$
$$\nabla x_5 = 0$$
$$\nabla x_6 = -e_3$$

$$\nabla x_7 = \nabla f(x) = \frac{\partial x_7}{\partial x_4} \nabla x_4 + \frac{\partial x_7}{\partial x_6} \nabla x_6 + \frac{\partial x_7}{\partial x_3} \nabla x_3 = \begin{bmatrix} 4 \\ \pi \\ 0 \end{bmatrix} - e_3 + e_3 = \begin{bmatrix} 4 \\ \pi \\ 0 \end{bmatrix}$$

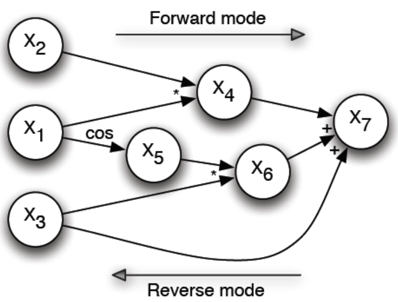


Variables	Derivatives
$x_4 = x_1 x_2$	$\frac{\partial x_4}{\partial x_1} = x_2, \frac{\partial x_4}{\partial x_2} = x_1$
$x_5 = \cos(x_1)$	$\frac{\partial x_5}{\partial x_1} = -\sin(x_1)$
$x_6 = x_5 x_3$	$\frac{\partial x_6}{\partial x_3} = x_5, \frac{\partial x_6}{\partial x_5} = x_3$
$x_7 = x_4 + x_6 + x_3$	$\frac{\partial x_7}{\partial x_3} = \frac{\partial x_7}{\partial x_4} = \frac{\partial x_7}{\partial x_6} = 1$

AD – forward and reverse

- Forward mode
  - Both x_i and ∇x_i are calculated by forward traversing computation graph

$$f(x_1, x_2, x_3) = x_1 x_2 + x_3 \cos(x_1) + x_3$$



Variables	Derivatives
$x_4 = x_1 x_2$	$\frac{\partial x_4}{\partial x_1} = x_2, \frac{\partial x_4}{\partial x_2} = x_1$
$x_5 = \cos(x_1)$	$\frac{\partial x_5}{\partial x_1} = -\sin(x_1)$
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$x_7 = x_4 + x_6 + x_3$	$\frac{\partial x_7}{\partial x_3} = \frac{\partial x_7}{\partial x_4} = \frac{\partial x_7}{\partial x_6} = 1$

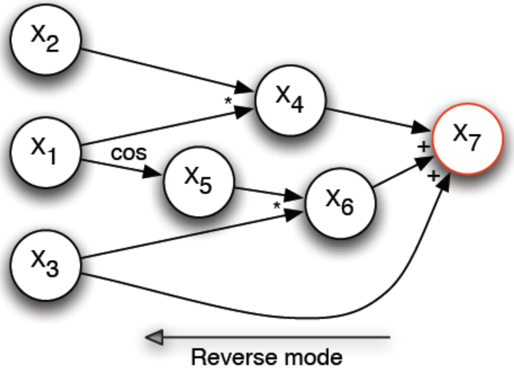
  - Reverse mode
    - First, calculate x_i by traversing graph forward
    - Then, calculate derivatives by traversing graph backward

AD – reverse mode

$$f(x_1, x_2, x_3) = x_1 x_2 + x_3 \cos(x_1) + x_3$$

$$x = (\pi, 4, 3)^\top$$

$$\frac{\partial f}{\partial x_7} = \frac{\partial x_7}{\partial x_7} = 1$$



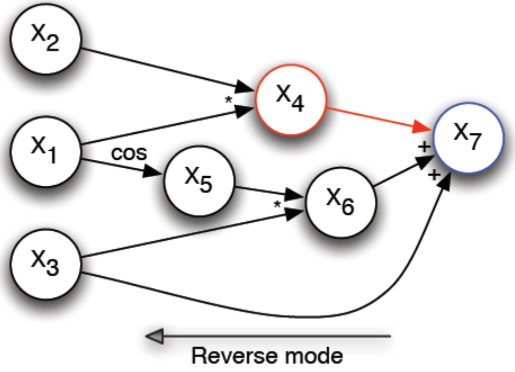
$$\frac{\partial f}{\partial x_i} = \sum_{x_n \text{ child of } x_i} \frac{\partial f}{\partial x_n} \frac{\partial x_n}{\partial x_i}$$

Variables	Derivatives
$x_4 = x_1 x_2$	$\frac{\partial x_4}{\partial x_1} = x_2, \frac{\partial x_4}{\partial x_2} = x_1$
$x_5 = \cos(x_1)$	$\frac{\partial x_5}{\partial x_1} = -\sin(x_1)$
$x_6 = x_5 x_3$	$\frac{\partial x_6}{\partial x_3} = x_5, \frac{\partial x_6}{\partial x_5} = x_3$
$x_7 = x_4 + x_6 + x_3$	$\frac{\partial x_7}{\partial x_3} = \frac{\partial x_7}{\partial x_4} = \frac{\partial x_7}{\partial x_6} = 1$

AD – reverse mode

$$f(x_1, x_2, x_3) = x_1 x_2 + x_3 \cos(x_1) + x_3$$
$$x = (\pi, 4, 3)^\top$$

$$\frac{\partial f}{\partial x_7} = \frac{\partial x_7}{\partial x_7} = 1$$
$$\frac{\partial f}{\partial x_4} = \frac{\partial f}{\partial x_7}\frac{\partial x_7}{\partial x_4} = 1$$



Variables	Derivatives
$x_4 = x_1 x_2$	$\frac{\partial x_4}{\partial x_1} = x_2, \frac{\partial x_4}{\partial x_2} = x_1$
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$x_7 = x_4 + x_6 + x_3$	$\frac{\partial x_7}{\partial x_3} = \frac{\partial x_7}{\partial x_4} = \frac{\partial x_7}{\partial x_6} = 1$

AD – reverse mode

$$f(x_1, x_2, x_3) = x_1 x_2 + x_3 \cos(x_1) + x_3$$

$$x = (\pi, 4, 3)^\top$$

$$\frac{\partial f}{\partial x_7} = \frac{\partial x_7}{\partial x_7} = 1$$
$$\frac{\partial f}{\partial x_4} = \frac{\partial f}{\partial x_7}\frac{\partial x_7}{\partial x_4} = 1$$
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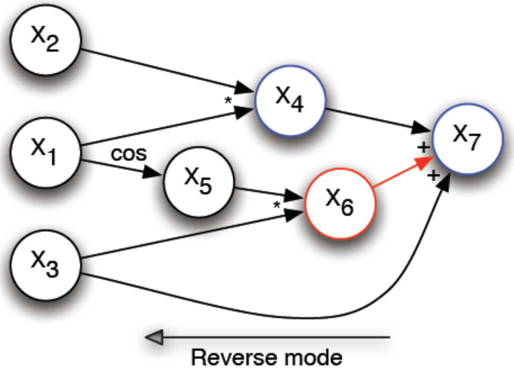

Variables	Derivatives
$x_4 = x_1 x_2$	$\frac{\partial x_4}{\partial x_1} = x_2, \frac{\partial x_4}{\partial x_2} = x_1$
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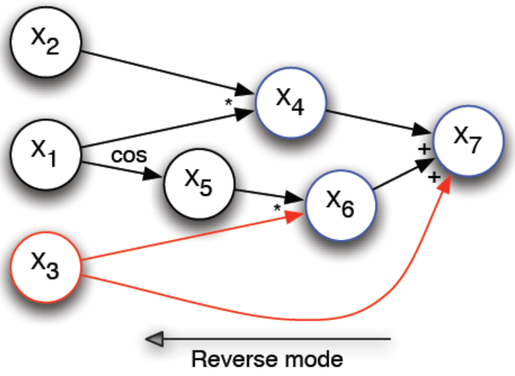
$x_7 = x_4 + x_6 + x_3$	$\frac{\partial x_7}{\partial x_3} = \frac{\partial x_7}{\partial x_4} = \frac{\partial x_7}{\partial x_6} = 1$

AD – reverse mode

$$f(x_1, x_2, x_3) = x_1 x_2 + x_3 \cos(x_1) + x_3$$
$$x = (\pi, 4, 3)^\top$$

$$\frac{\partial f}{\partial x_7} = \frac{\partial x_7}{\partial x_7} = 1$$
$$\frac{\partial f}{\partial x_4} = \frac{\partial f}{\partial x_7}\frac{\partial x_7}{\partial x_4} = 1$$
$$\frac{\partial f}{\partial x_6} = \frac{\partial f}{\partial x_7}\frac{\partial x_7}{\partial x_6} = 1$$
$$\frac{\partial f}{\partial x_3} = \frac{\partial f}{\partial x_7}\frac{\partial x_7}{\partial x_3} + \frac{\partial f}{\partial x_6}\frac{\partial x_6}{\partial x_3} = 1 + x_5 = 1 + \cos(\pi) = 0$$



Variables	Derivatives
$x_4 = x_1 x_2$	$\frac{\partial x_4}{\partial x_1} = x_2, \frac{\partial x_4}{\partial x_2} = x_1$
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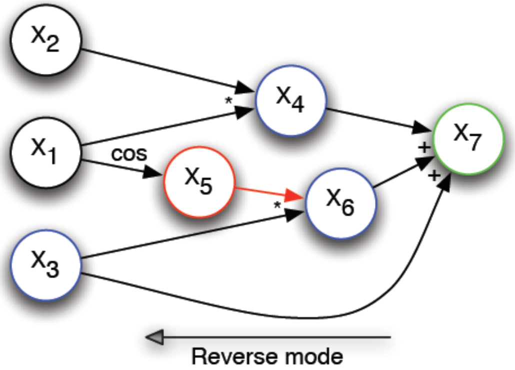
$x_7 = x_4 + x_6 + x_3$	$\frac{\partial x_7}{\partial x_3} = \frac{\partial x_7}{\partial x_4} = \frac{\partial x_7}{\partial x_6} = 1$

AD – reverse mode

$$f(x_1, x_2, x_3) = x_1 x_2 + x_3 \cos(x_1) + x_3$$
$$x = (\pi, 4, 3)^\top$$

$$\frac{\partial f}{\partial x_7} = \frac{\partial x_7}{\partial x_7} = 1$$
$$\frac{\partial f}{\partial x_4} = \frac{\partial f}{\partial x_7}\frac{\partial x_7}{\partial x_4} = 1$$
$$\frac{\partial f}{\partial x_6} = \frac{\partial f}{\partial x_7}\frac{\partial x_7}{\partial x_6} = 1$$
$$\frac{\partial f}{\partial x_3} = \frac{\partial f}{\partial x_7}\frac{\partial x_7}{\partial x_3} + \frac{\partial f}{\partial x_6}\frac{\partial x_6}{\partial x_3} = 1 + x_5 = 1 + \cos(\pi) = 0$$
$$\frac{\partial f}{\partial x_5} = \frac{\partial f}{\partial x_6}\frac{\partial x_6}{\partial x_5} = x_3 = 3$$



Variables	Derivatives
$x_4 = x_1 x_2$	$\frac{\partial x_4}{\partial x_1} = x_2, \frac{\partial x_4}{\partial x_2} = x_1$
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$x_7 = x_4 + x_6 + x_3$	$\frac{\partial x_7}{\partial x_3} = \frac{\partial x_7}{\partial x_4} = \frac{\partial x_7}{\partial x_6} = 1$

AD – reverse mode

$$f(x_1, x_2, x_3) = x_1 x_2 + x_3 \cos(x_1) + x_3$$

$$x = (\pi, 4, 3)^\top$$

$$\frac{\partial f}{\partial x_7} = \frac{\partial x_7}{\partial x_7} = 1$$

$$\frac{\partial f}{\partial x_4} = \frac{\partial f}{\partial x_7}\frac{\partial x_7}{\partial x_4} = 1$$

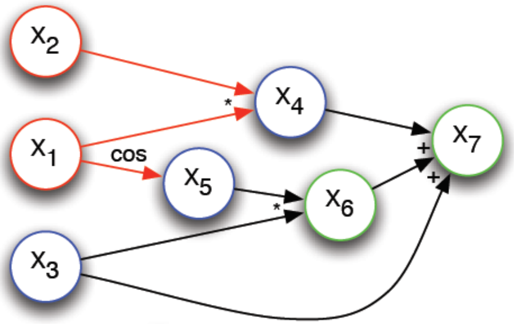
$$\frac{\partial f}{\partial x_6} = \frac{\partial f}{\partial x_7}\frac{\partial x_7}{\partial x_6} = 1$$

$$\frac{\partial f}{\partial x_3} = \frac{\partial f}{\partial x_7}\frac{\partial x_7}{\partial x_3} + \frac{\partial f}{\partial x_6}\frac{\partial x_6}{\partial x_3} = 1 + x_5 = 1 + \cos(\pi) = \underline{0}$$

$$\frac{\partial f}{\partial x_5} = \frac{\partial f}{\partial x_6}\frac{\partial x_6}{\partial x_5} = x_3 = 3$$

$$\frac{\partial f}{\partial x_1} = \frac{\partial f}{\partial x_4}\frac{\partial x_4}{\partial x_1} + \frac{\partial f}{\partial x_5}\frac{\partial x_5}{\partial x_1} = x_2 - 3\sin(x_1) = 4 - 3\sin(\pi) = \underline{4}$$

$$\frac{\partial f}{\partial x_2} = \frac{\partial f}{\partial x_4}\frac{\partial x_4}{\partial x_2} = x_1 = \underline{\pi}$$



Variables	Derivatives
$x_4 = x_1 x_2$	$\frac{\partial x_4}{\partial x_1} = x_2, \frac{\partial x_4}{\partial x_2} = x_1$
$x_5 = \cos(x_1)$	$\frac{\partial x_5}{\partial x_1} = -\sin(x_1)$
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$x_7 = x_4 + x_6 + x_3$	$\frac{\partial x_7}{\partial x_3} = \frac{\partial x_7}{\partial x_4} = \frac{\partial x_7}{\partial x_6} = 1$

Example: optimization using CasADi

- CasADi (https://casadi.org/)
  - “CasADi is a symbolic framework for numeric optimization implementing automatic differentiation in forward and reverse modes on sparse matrix-valued computational graphs.”

$$\min_{x,y,z} \quad x^2 + 100z^2 \qquad f(x,y,z)$$

$$\text{s.t.} \quad z + (1-x)^2 - y = 0$$

$g(x,y,z) = 0$

Define variables

Define objective and constraints

Create solver object

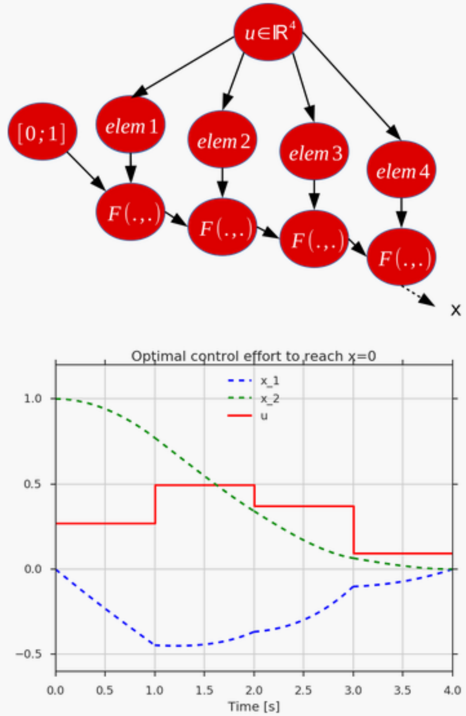
Solve the opt problem

rosenbrock.m

```
import casadi.*

% Create NLP: Solve the Rosenbrock problem:
%     minimize    x^2 + 100*z^2
%     subject to  z + (1-x)^2 - y == 0
x = SX.sym('x');
y = SX.sym('y');
z = SX.sym('z');
v = [x;y;z];
f = x^2 + 100*z^2;
g = z + (1-x)^2 - y;
nlp = struct('x', v, 'f', f, 'g', g);

% Create IPOPT solver object
solver = nlpsol('solver', 'ipopt', nlp);

% Solve the NLP
res = solver('x0' , [2.5 3.0 0.75],... % solution guess
             'lbx', -inf,...            % lower bound on x
             'ubx',  inf,...            % upper bound on x
             'lbg',    0,...            % lower bound on g
             'ubg',    0);              % upper bound on g

% Print the solution
f_opt = full(res.f)          % >> 0
x_opt = full(res.x)          % >> [0; 1; 0]
lam_x_opt = full(res.lam_x)  % >> [0; 0; 0]
lam_g_opt = full(res.lam_g)  % >> 0
```

Example from CasADi

Example | Octave/Matlab | Python | C++

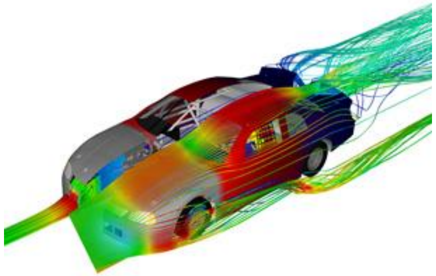


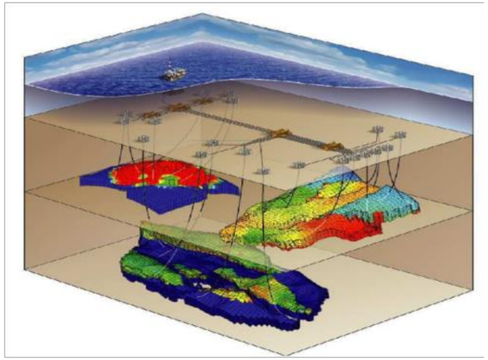
Example | Octave/Matlab | **Python** | C++

```python
from casadi import *


x = MX.sym('x',2); # Two states
p = MX.sym('p');   # Free parameter

# Expression for ODE right-hand side
z = 1-x[1]**2;
rhs = vertcat(z*x[0]-x[1]+2*tanh(p),x[0])

# ODE declaration with free parameter
ode = {'x':x,'p':p,'ode':rhs}

# Construct a Function that integrates over 1s
F = integrator('F','cvodes',ode,{'tf':1})

# Control vector
u = MX.sym('u',4,1)

x = [0,1]  # Initial state
for k in range(4):
  # Integrate 1s forward in time:
  # call integrator symbolically
  res = F(x0=x,p=u[k])
  x = res["xf"]


# NLP declaration
nlp = {'x':u,'f':dot(u,u),'g':x};

# Solve using IPOPT
solver = nlpsol('solver','ipopt',nlp)
res = solver(x0=0.2,lbg=0,ubg=0)

plot(res["x"])
```

Derivative-free optimization

- If you have derivatives (gradients, possibly Hessian), use them!
  - "Always" more efficient than not using them!
- However, sometimes, obtaining derivatives is prohibitive
  - Typically: Objective function (and constraints) are calculated using "heavy" simulators
    - Often models from computational fluid dynamics (CFD)



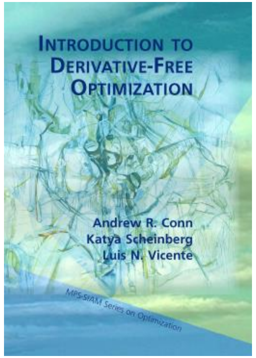


- (Or you are optimizing a "real" system without a model!)

- This motivates "derivative-free optimization" methods

Derivative-free optimization (DFO)

- DFO use function values at a set of sample points to determine new iterates.
- Coarsely, two different classes of methods:
  1. “Model-based”: sample points -> approximate model -> search directions
  2. “Metaheuristics”: Often inspired by processes in nature, such as “genetic algorithm”, “simulated annealing”, “particle swarm optimization”, “wolf pack optimization”, …

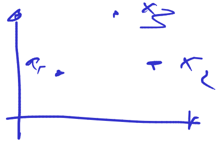


- Many of the metaheuristic methods claim to do “global optimization” and tackle “non-differentiable problems”, however: Guarantees are seldom given.
- The “model-based” methods are based on a solid theoretic framework, and are generally preferable (in my opinion)

- But for all methods:
  - **DFO generally works best if the number of optimization variables is relatively small**

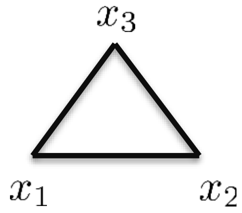
- Here: Nelder-Mead (old&simple, but OK)

Nelder-Mead Simplex method (Ch. 9.5)

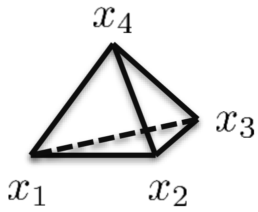


$\min_{x \in \mathbb{R}^n} f(x)$ – can evaluate $f(x)$, but not $\nabla f(x)$

"simplex" : "generalized triangle"



Simplex 2D



Simplex 3D

starting point:

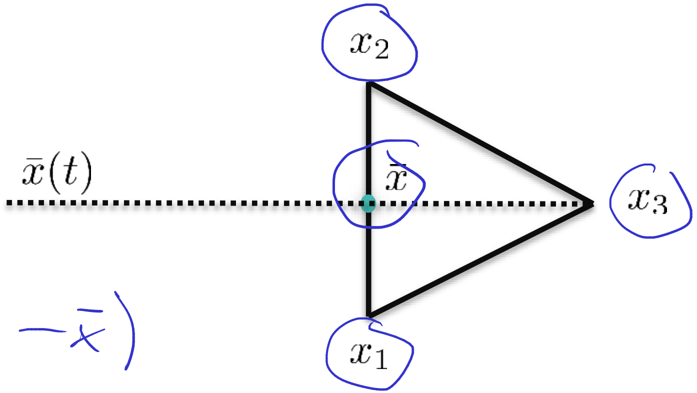
- Initial simplex: $S = \{x_1, x_2, \dots, x_{n+1}\}$
- Matrix $V(S) = [x_2 - x_1, x_3 - x_1, \dots, x_{n+1} - x_1]$ is non-singular
- ordered vertices:

$f(x_1) \le f(x_2) \le \dots \le f(x_{n+1})$

Nelder-Mead Simplex method (Ch. 9.5)

Define centroid of best n points

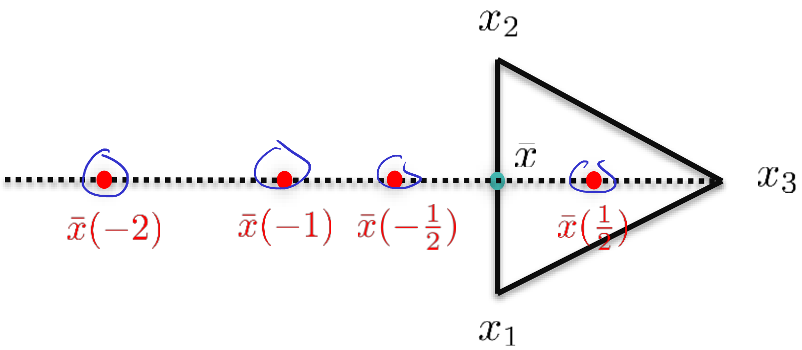
$$\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$$



Define line: $\underline{\bar{x}(t)} = \bar{x} + t(x_{n+1} - \bar{x})$

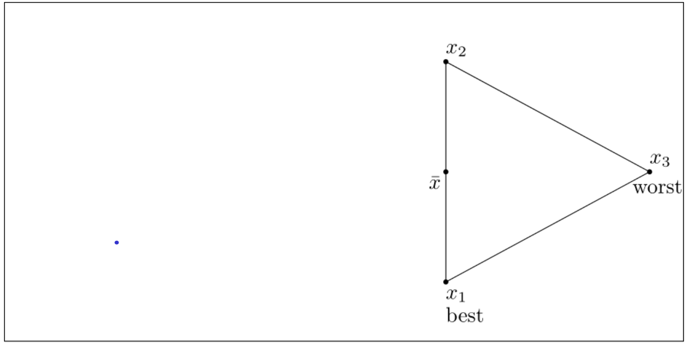
One iteration of Nelder-Mead

$$\bar{x}(t) = \bar{x} + t\,(x_{n+1} - \bar{x})$$



One iteration of Nelder-Mead

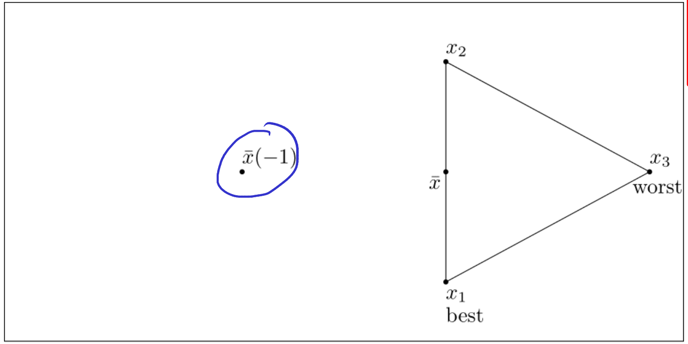
$n+1$ vertices $\{x_1, x_2, \ldots, x_{n+1}\}$ of *nonsingular* simplex, ordered such that $f(x_1) \le f(x_2) \le \ldots \le f(x_{n+1})$
Define centroid of n best points, $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$.
Define $\bar{x}(t) = \bar{x} + t(x_{n+1} - \bar{x})$



Compute $\bar{x}(-1)$ and evaluate $f_{-1} = f(\bar{x}(-1))$
  if $f(x_1) \le f_{-1} < f(x_n)$ "$\bar{x}(-1)$ is OK"
    replace x_{n+1} by $\bar{x}(-1)$, go to next iteration.
  else if $f_{-1} < f(x_1)$ "$\bar{x}(-1)$ is great, try further"
    evaluate $f_{-2} = f(\bar{x}(-2))$
    if $f_{-2} < f_{-1}$
      replace x_{n+1} by $\bar{x}(-2)$, go to next iteration.
    else
      replace x_{n+1} by $\bar{x}(-1)$, go to next iteration.
  else if $f_{-1} \ge f(x_n)$ "$\bar{x}(-1)$ is bad"
    if $f(x_n) \le f_{-1} < f(x_{n+1})$
      evaluate $f_{-1/2} = f(\bar{x}(-1/2))$
      if $f_{-1/2} \le f_{-1}$
        replace x_{n+1} by $\bar{x}(-1/2)$, go to next iteration.
    else $(f_{-1} > f(x_{n+1}))$
      evaluate $f_{1/2} = f(\bar{x}(1/2))$
      if $f_{1/2} < f_{n+1}$
        replace x_{n+1} by $\bar{x}(1/2)$, go to next iteration.
    replace $x_i \leftarrow \frac{1}{2}(x_1 + x_i)$, $i = 2, 3, \ldots, n+1$ "shrink"

One iteration of Nelder-Mead

$n+1$ vertices $\{x_1, x_2, \ldots, x_{n+1}\}$ of *nonsingular* simplex, ordered such that $f(x_1) \leq f(x_2) \leq \ldots \leq f(x_{n+1})$
Define centroid of n best points, $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$.
Define $\bar{x}(t) = \bar{x} + t(x_{n+1} - \bar{x})$

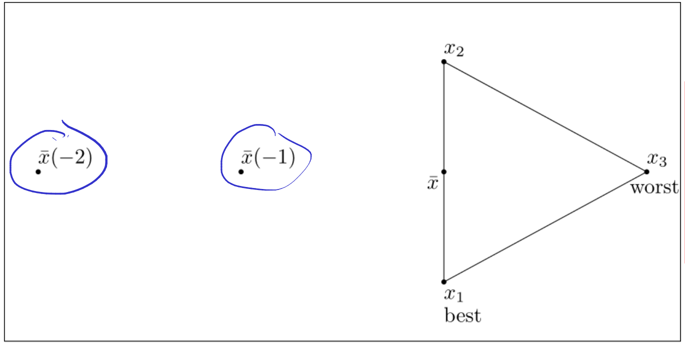


Reflection

Compute $\bar{x}(-1)$ and evaluate $f_{-1} = f(\bar{x}(-1))$
  if $f(x_1) \leq f_{-1} < f(x_n)$ "$\bar{x}(-1)$ is OK"
    replace x_{n+1} by $\bar{x}(-1)$, go to next iteration.
  else if $f_{-1} < f(x_1)$ "$\bar{x}(-1)$ is great, try further"
    evaluate $f_{-2} = f(\bar{x}(-2))$
    if $f_{-2} < f_{-1}$
      replace x_{n+1} by $\bar{x}(-2)$, go to next iteration.
    else
      replace x_{n+1} by $\bar{x}(-1)$, go to next iteration.
  else if $f_{-1} \geq f(x_n)$ "$\bar{x}(-1)$ is bad"
    if $f(x_n) \leq f_{-1} < f(x_{n+1})$
      evaluate $f_{-1/2} = f(\bar{x}(-1/2))$
      if $f_{-1/2} \leq f_{-1}$
        replace x_{n+1} by $\bar{x}(-1/2)$, go to next iteration.
    else $(f_{-1} > f(x_{n+1}))$
      evaluate $f_{1/2} = f(\bar{x}(1/2))$
      if $f_{1/2} < f_{n+1}$
        replace x_{n+1} by $\bar{x}(1/2)$, go to next iteration.
    replace $x_i \leftarrow \frac{1}{2}(x_1 + x_i)$, $i = 2, 3, \ldots, n+1$ "shrink"

One iteration of Nelder-Mead

$n+1$ vertices $\{x_1, x_2, \ldots, x_{n+1}\}$ of *nonsingular* simplex, ordered such that $f(x_1) \leq f(x_2) \leq \ldots \leq f(x_{n+1})$
Define centroid of n best points, $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$.
Define $\bar{x}(t) = \bar{x} + t(x_{n+1} - \bar{x})$

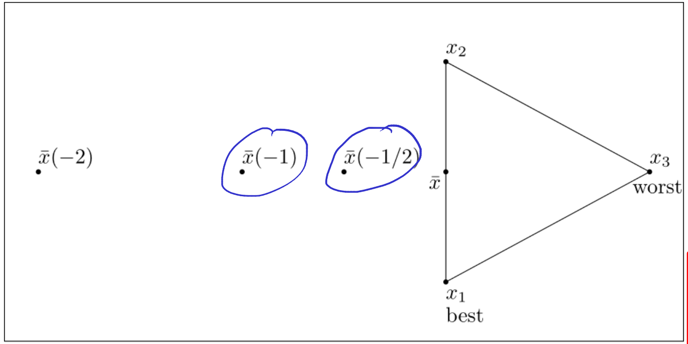


Expansion

Compute $\bar{x}(-1)$ and evaluate $f_{-1} = f(\bar{x}(-1))$
 if $f(x_1) \leq f_{-1} < f(x_n)$ "$\bar{x}(-1)$ is OK"
  replace x_{n+1} by $\bar{x}(-1)$, go to next iteration.
 else if $f_{-1} < f(x_1)$ "$\bar{x}(-1)$ is great, try further"
  evaluate $f_{-2} = f(\bar{x}(-2))$
  if $f_{-2} < f_{-1}$
   replace x_{n+1} by $\bar{x}(-2)$, go to next iteration.
  else
   replace x_{n+1} by $\bar{x}(-1)$, go to next iteration.
 else if $f_{-1} \geq f(x_n)$ "$\bar{x}(-1)$ is bad"
  if $f(x_n) \leq f_{-1} < f(x_{n+1})$
   evaluate $f_{-1/2} = f(\bar{x}(-1/2))$
   if $f_{-1/2} \leq f_{-1}$
    replace x_{n+1} by $\bar{x}(-1/2)$, go to next iteration.
  else $(f_{-1} > f(x_{n+1}))$
   evaluate $f_{1/2} = f(\bar{x}(1/2))$
   if $f_{1/2} < f_{n+1}$
    replace x_{n+1} by $\bar{x}(1/2)$, go to next iteration.
  replace $x_i \leftarrow \frac{1}{2}(x_1 + x_i)$, $i = 2, 3, \ldots, n+1$ "shrink"

One iteration of Nelder-Mead

$n+1$ vertices $\{x_1, x_2, \ldots, x_{n+1}\}$ of *nonsingular* simplex, ordered such that $f(x_1) \le f(x_2) \le \ldots \le f(x_{n+1})$
Define centroid of n best points, $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$.
Define $\bar{x}(t) = \bar{x} + t(x_{n+1} - \bar{x})$

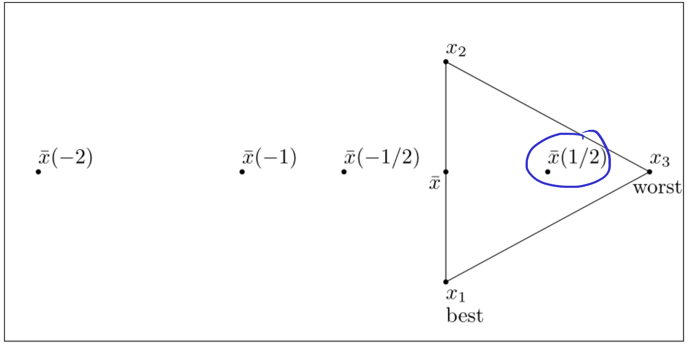


Contraction (outside)

Compute $\bar{x}(-1)$ and evaluate $f_{-1} = f(\bar{x}(-1))$
if $f(x_1) \le f_{-1} < f(x_n)$ "$\bar{x}(-1)$ is OK"
  replace x_{n+1} by $\bar{x}(-1)$, go to next iteration.
else if $f_{-1} < f(x_1)$ "$\bar{x}(-1)$ is great, try further"
  evaluate $f_{-2} = f(\bar{x}(-2))$
  if $f_{-2} < f_{-1}$
    replace x_{n+1} by $\bar{x}(-2)$, go to next iteration.
  else
    replace x_{n+1} by $\bar{x}(-1)$, go to next iteration.
else if $f_{-1} \ge f(x_n)$ "$\bar{x}(-1)$ is bad"
  if $f(x_n) \le f_{-1} < f(x_{n+1})$
    evaluate $f_{-1/2} = f(\bar{x}(-1/2))$
    if $f_{-1/2} \le f_{-1}$
      replace x_{n+1} by $\bar{x}(-1/2)$, go to next iteration.
  else $(f_{-1} > f(x_{n+1}))$
    evaluate $f_{1/2} = f(\bar{x}(1/2))$
    if $f_{1/2} < f_{n+1}$
      replace x_{n+1} by $\bar{x}(1/2)$, go to next iteration.
  replace $x_i \leftarrow \frac{1}{2}(x_1 + x_i)$, $i = 2, 3, \ldots, n+1$ "shrink"

One iteration of Nelder-Mead

$n+1$ vertices $\{x_1, x_2, \ldots, x_{n+1}\}$ of *nonsingular* simplex, ordered such that $f(x_1) \le f(x_2) \le \ldots \le f(x_{n+1})$
Define centroid of n best points, $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$.
Define $\bar{x}(t) = \bar{x} + t(x_{n+1} - \bar{x})$

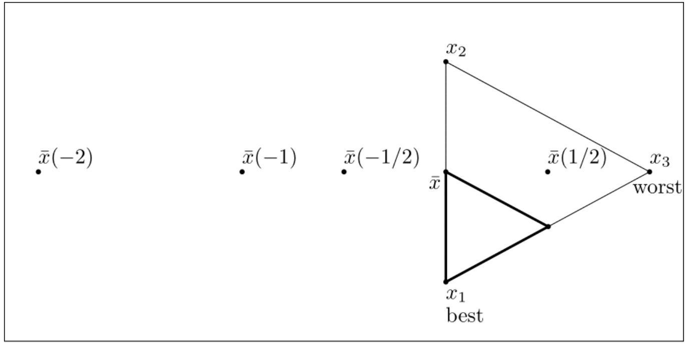


Contraction (inside)

Compute $\bar{x}(-1)$ and evaluate $f_{-1} = f(\bar{x}(-1))$
- **if** $f(x_1) \le f_{-1} < f(x_n)$ "$\bar{x}(-1)$ is OK"
  - replace x_{n+1} by $\bar{x}(-1)$, go to next iteration.
- **else if** $f_{-1} < f(x_1)$ "$\bar{x}(-1)$ is great, try further"
  - evaluate $f_{-2} = f(\bar{x}(-2))$
  - **if** $f_{-2} < f_{-1}$
    - replace x_{n+1} by $\bar{x}(-2)$, go to next iteration.
  - **else**
    - replace x_{n+1} by $\bar{x}(-1)$, go to next iteration.
- **else if** $f_{-1} \ge f(x_n)$ "$\bar{x}(-1)$ is bad"
  - **if** $f(x_n) \le f_{-1} < f(x_{n+1})$
    - evaluate $f_{-1/2} = f(\bar{x}(-1/2))$
    - **if** $f_{-1/2} \le f_{-1}$
      - replace x_{n+1} by $\bar{x}(-1/2)$, go to next iteration.
  - **else** $(f_{-1} > f(x_{n+1}))$
    - evaluate $f_{1/2} = f(\bar{x}(1/2))$
    - **if** $f_{1/2} < f_{n+1}$
      - replace x_{n+1} by $\bar{x}(1/2)$, go to next iteration.
  - replace $x_i \leftarrow \frac{1}{2}(x_1 + x_i)$, $i = 2, 3, \ldots, n+1$ "shrink"

One iteration of Nelder-Mead

$n+1$ vertices $\{x_1, x_2, \ldots, x_{n+1}\}$ of *nonsingular* simplex, ordered such that $f(x_1) \le f(x_2) \le \ldots \le f(x_{n+1})$
Define centroid of n best points, $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$.
Define $\bar{x}(t) = \bar{x} + t(x_{n+1} - \bar{x})$



Shrinkage

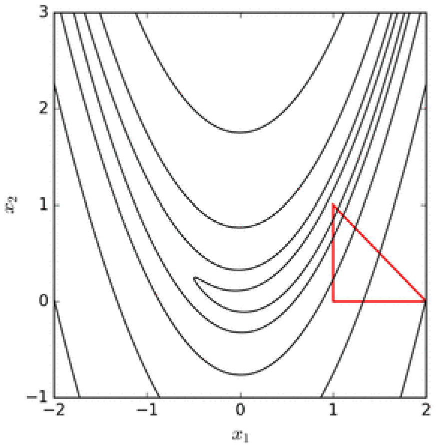
Compute $\bar{x}(-1)$ and evaluate $f_{-1} = f(\bar{x}(-1))$
- **if** $f(x_1) \le f_{-1} < f(x_n)$ "$\bar{x}(-1)$ is OK"
  - replace x_{n+1} by $\bar{x}(-1)$, go to next iteration.
- **else if** $f_{-1} < f(x_1)$ "$\bar{x}(-1)$ is great, try further"
  - evaluate $f_{-2} = f(\bar{x}(-2))$
  - **if** $f_{-2} < f_{-1}$
    - replace x_{n+1} by $\bar{x}(-2)$, go to next iteration.
  - **else**
    - replace x_{n+1} by $\bar{x}(-1)$, go to next iteration.
- **else if** $f_{-1} \ge f(x_n)$ "$\bar{x}(-1)$ is bad"
  - **if** $f(x_n) \le f_{-1} < f(x_{n+1})$
    - evaluate $f_{-1/2} = f(\bar{x}(-1/2))$
    - **if** $f_{-1/2} \le f_{-1}$
      - replace x_{n+1} by $\bar{x}(-1/2)$, go to next iteration.
  - **else** $(f_{-1} > f(x_{n+1}))$
    - evaluate $f_{1/2} = f(\bar{x}(1/2))$
    - **if** $f_{1/2} < f_{n+1}$
      - replace x_{n+1} by $\bar{x}(1/2)$, go to next iteration.
  - replace $x_i \leftarrow \frac{1}{2}(x_1 + x_i)$, $i = 2, 3, \ldots, n+1$ "shrink"

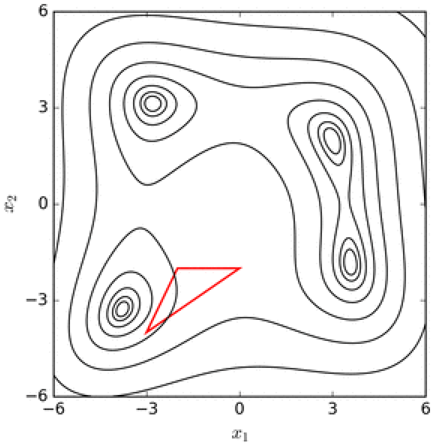
Termination and convergence

Termination: $|f(x_1) - f(x_{n+1})| \leq \text{tol}$

Convergence: The average value $\frac{1}{n+1}\sum_{i=1}^{n+1} f(x_i)$ decrease in most iterations

Examples





wikipedia.org

Three different DFO methods, three examples

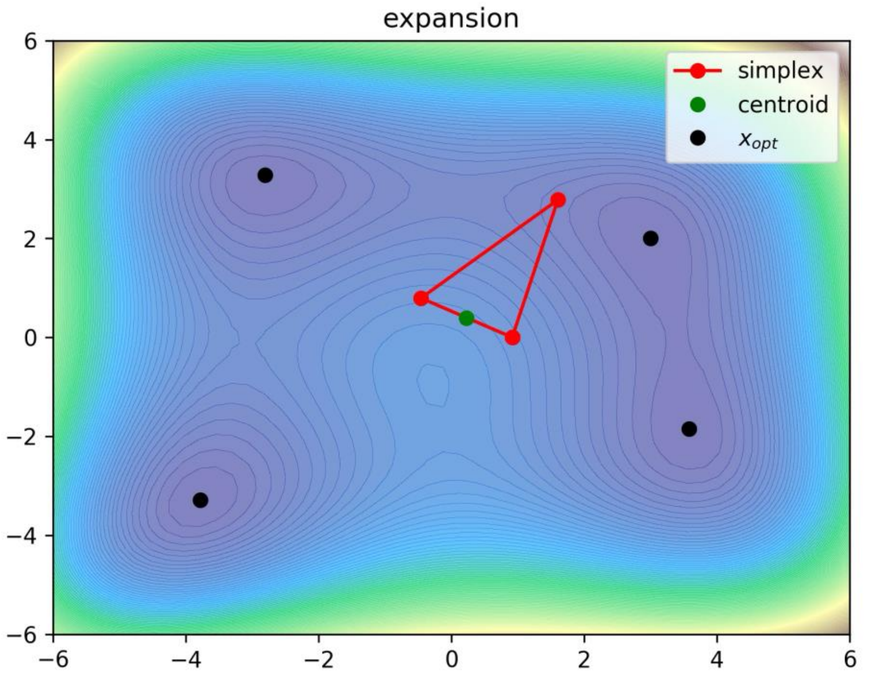
Methods:

- Nelder-Mead
- Coordinate descent
- Particle swarm (a metaheuristic method)

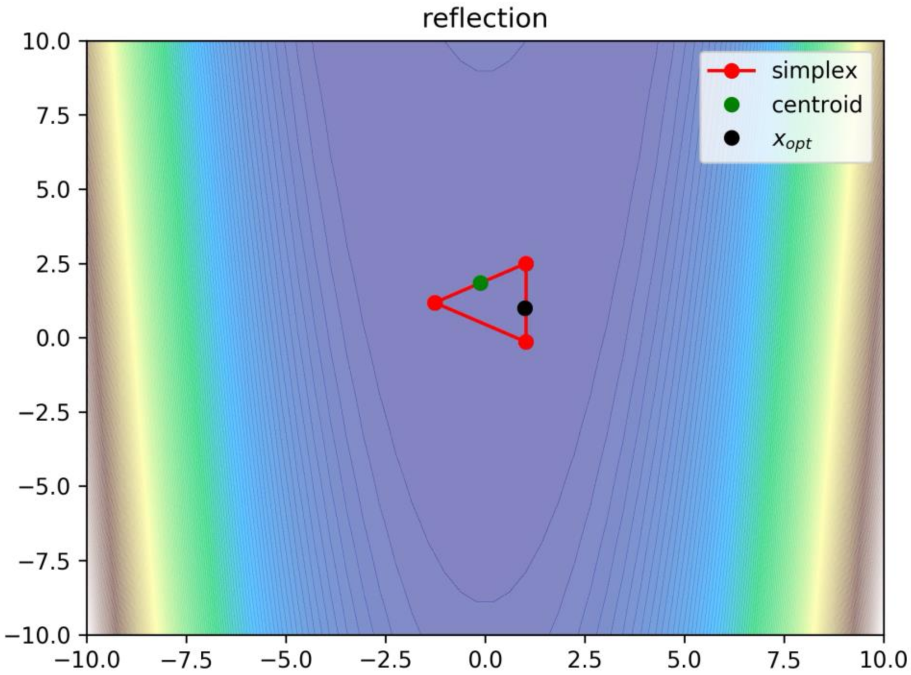
Examples

- Himmelblau (four local minimums, global min x = (3,2))
- Rosenbrock (one local/global minimum at x = (0,0))
- Salomon (many local minimums, global min x = (0,0))

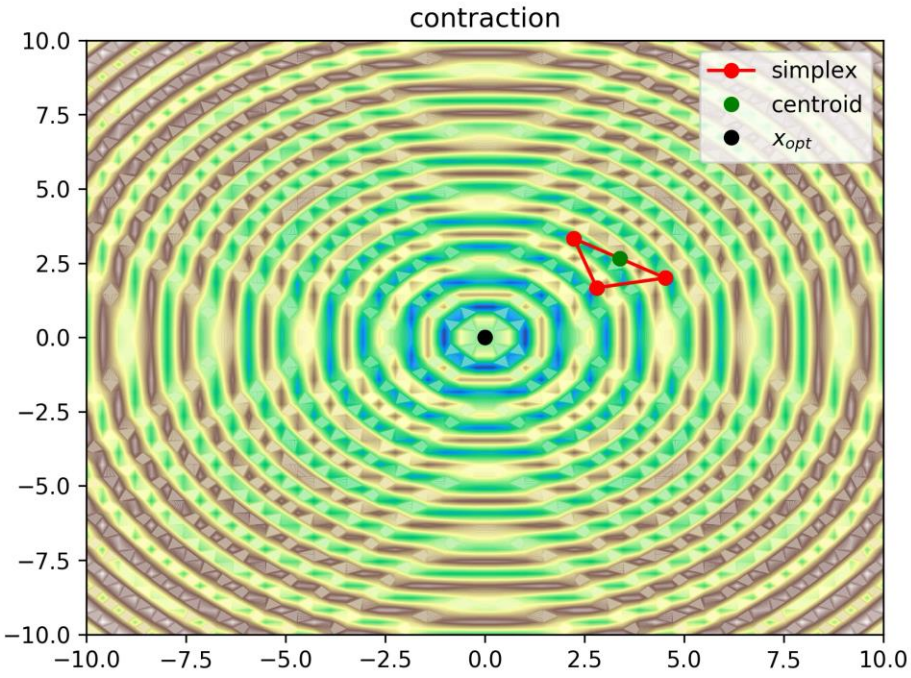
Examples: Nelder-Mead, Himmelblau



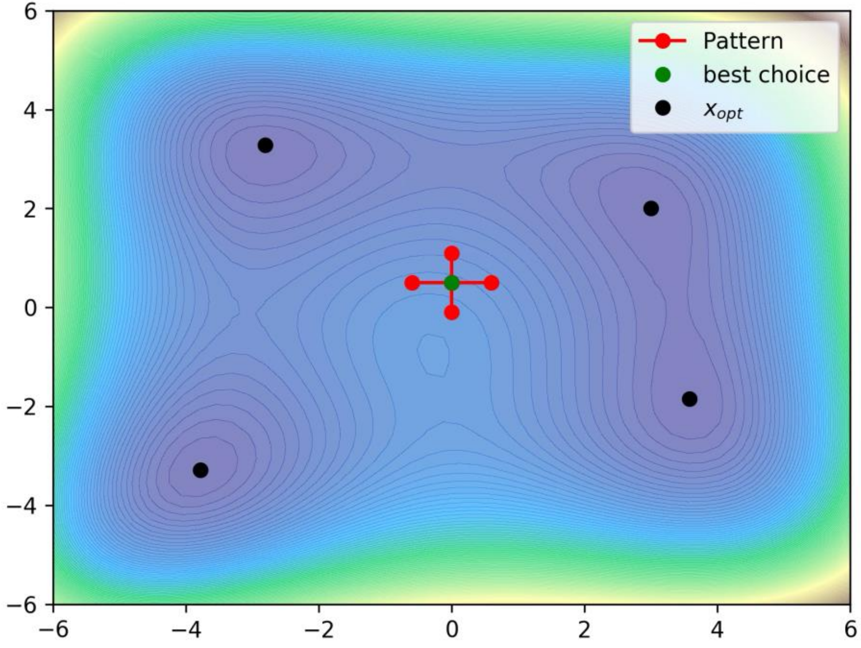
Example: Nelder-Mead, Rosenbrock



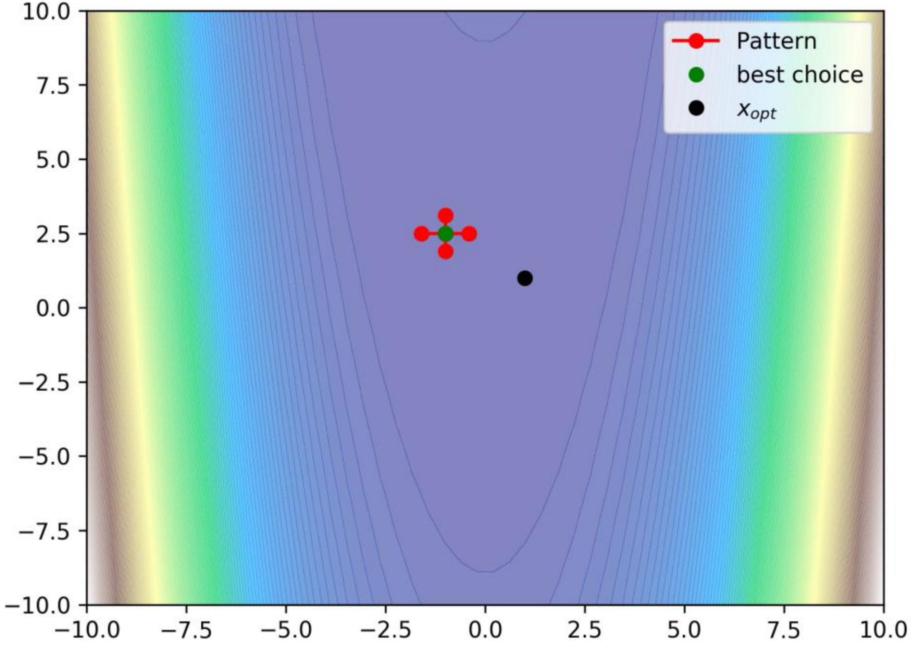
Example: Nelder-Mead, Salomon



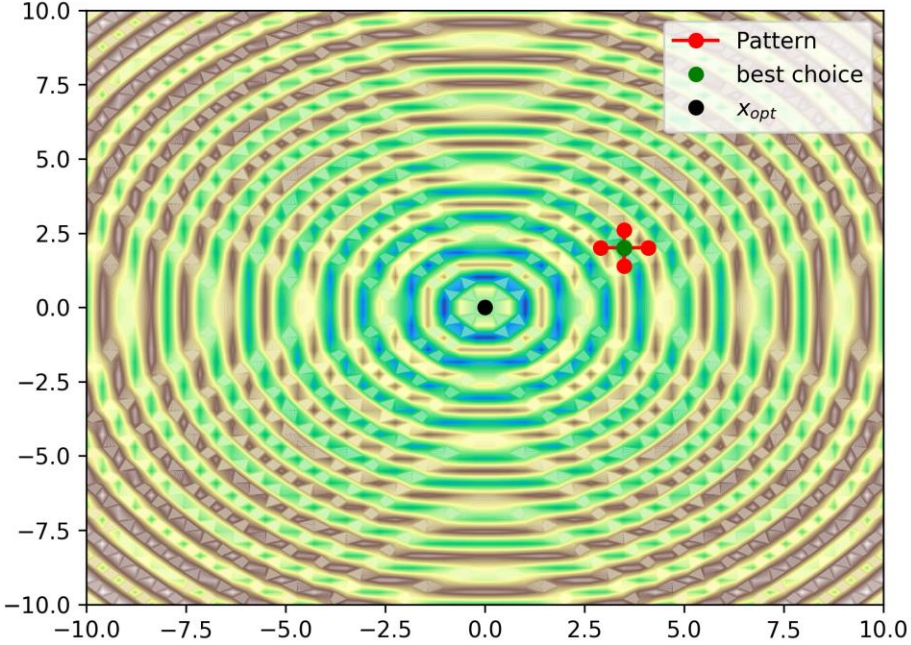
Example: Coordinate Descent, Himmelblau



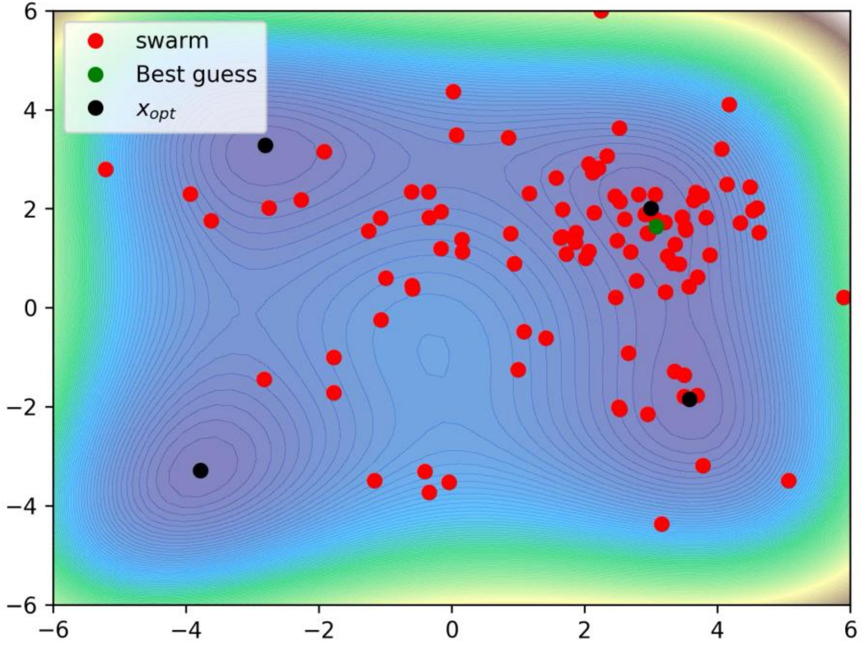
Example: Coordinate Descent, Rosenbrock



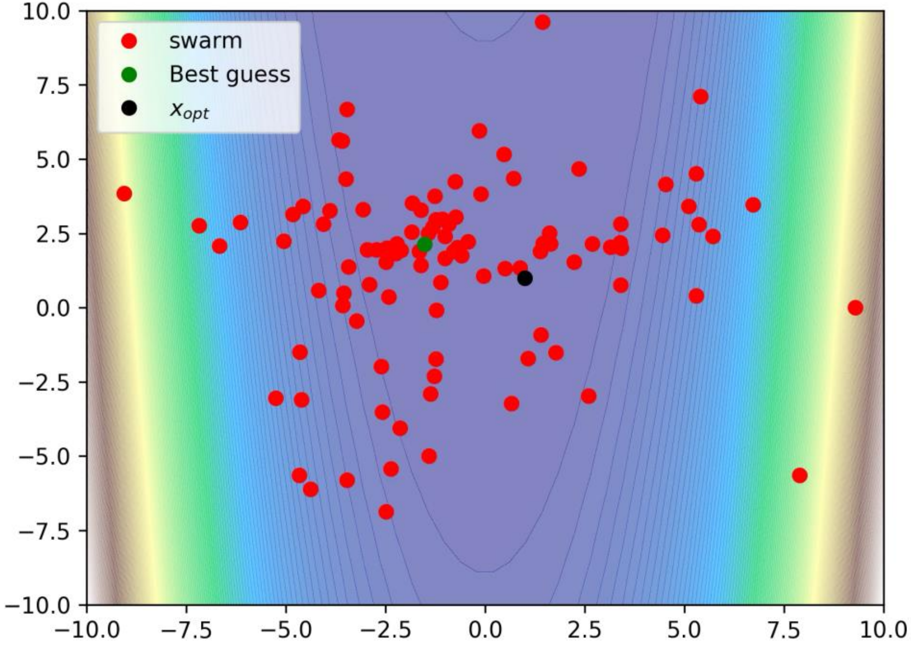
Example: Coordinate Descent, Salomon



Example: Particle Swarm, Himmelblau



Example: Particle Swarm, Rosenbrock



Example: Particle Swarm, Salomon