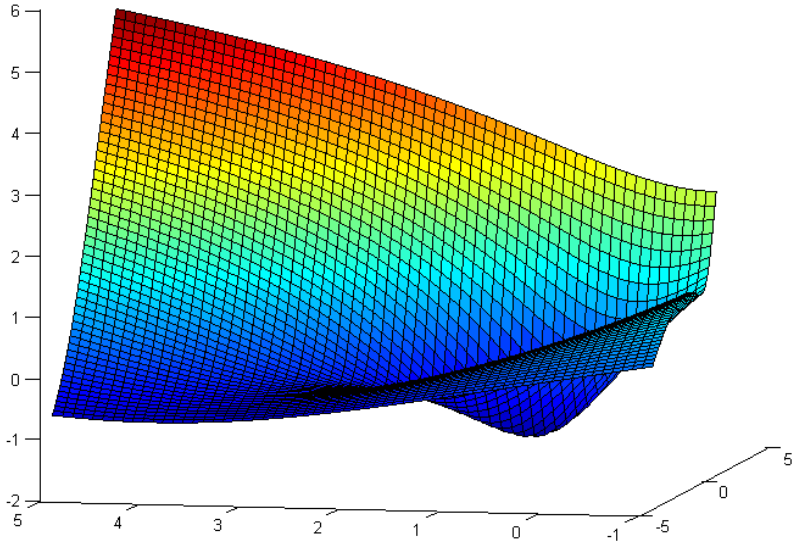
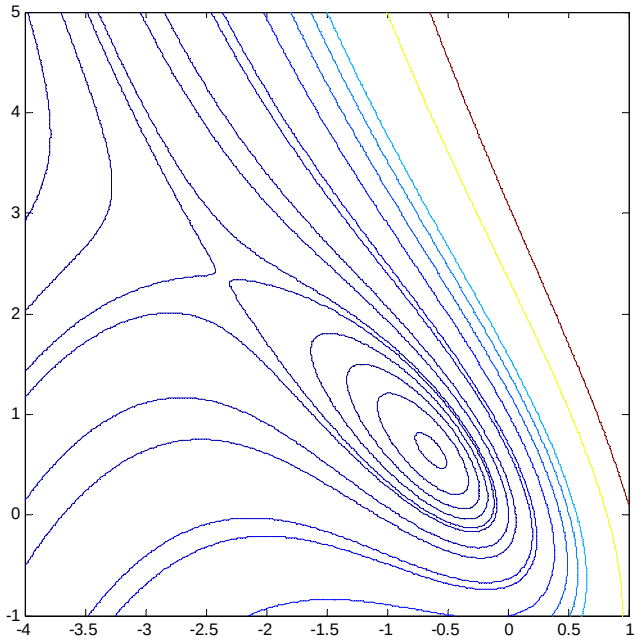
Lecture 2

- Newton's method
  - Line search
- Quasi-Newton methods
- Least-Squares and Gauss-Newton methods
- Downhill simplex (amoeba) algorithm

Optimization for General Functions

$$f(x,y) = \exp(x)(4x^2 + 2y^2 + 4xy + 2x + 1)$$

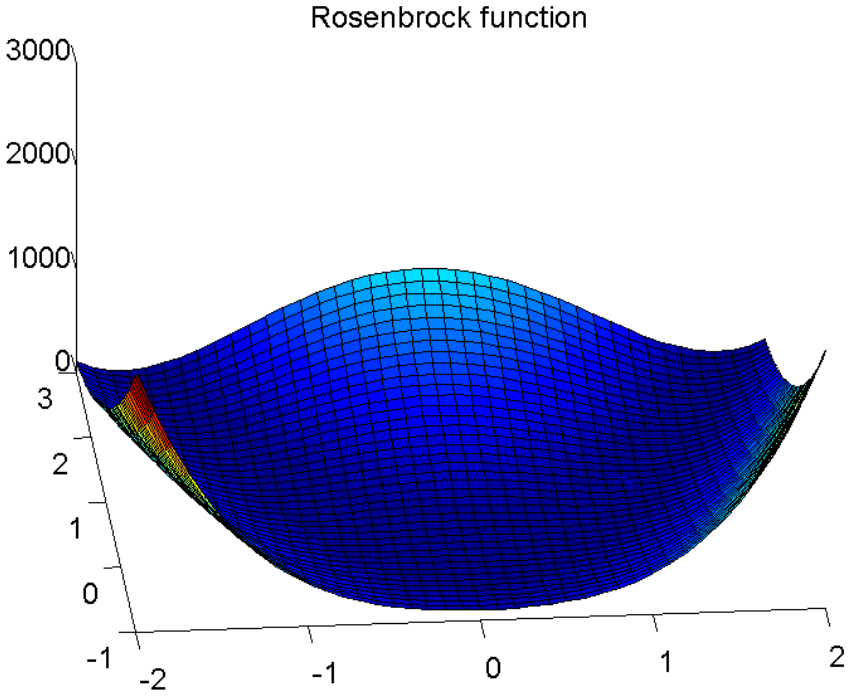


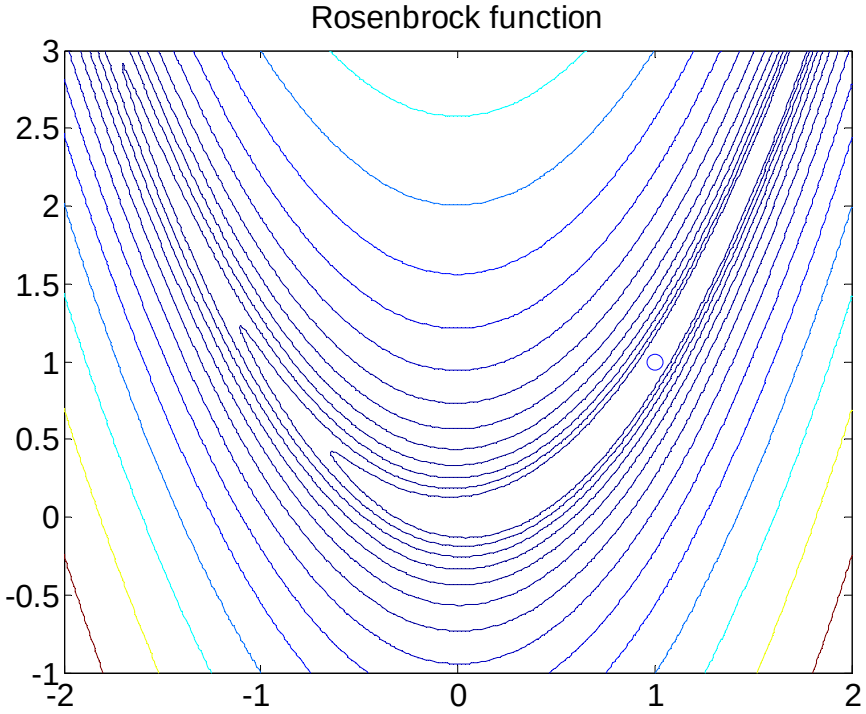


Apply methods developed using quadratic Taylor series expansion

Rosenbrock's function

$$f(x, y) = 100(y - x^2)^2 + (1 - x)^2$$

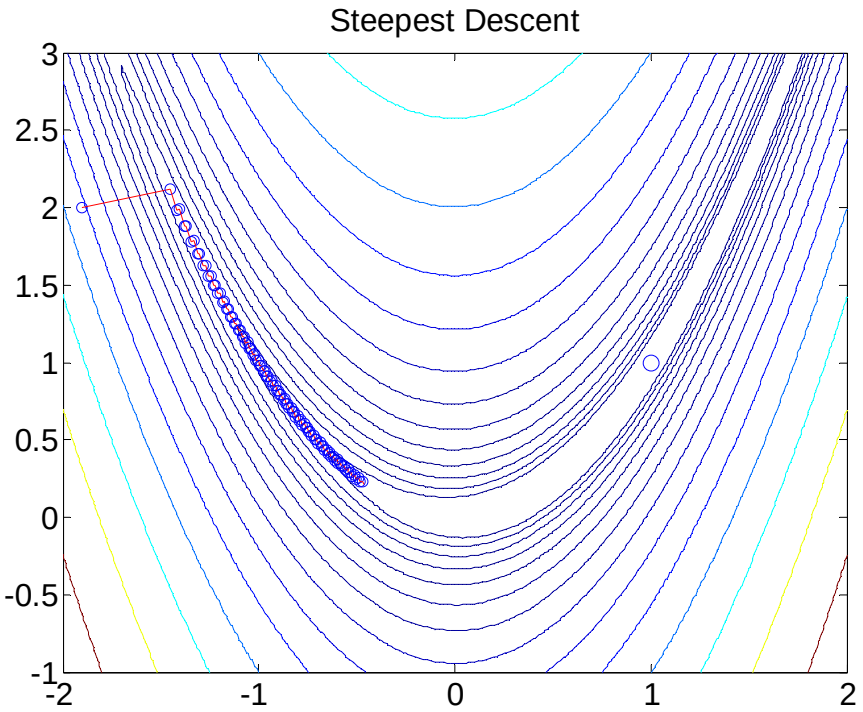


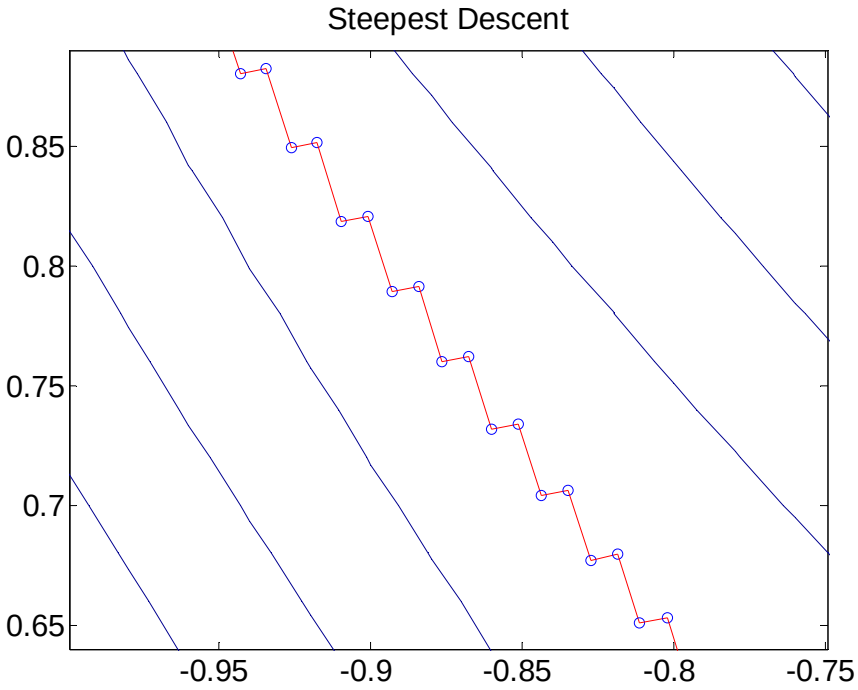


Minimum is at $[1, 1]$

Steepest descent

- The 1D line minimization must be performed using one of the earlier methods (usually cubic polynomial interpolation)





- The zig-zag behaviour is clear in the zoomed view (100 iterations)
- The algorithm crawls down the valley

Performance issues for optimization algorithms

1. Number of iterations required

2. Cost per iteration

3. Memory footprint

4. Region of convergence

Recall from lecture 1: Newton's method in 1D

Fit a quadratic approximation to $f(x)$ using both gradient and curvature information at $\mathbf{x}$.

- Expand $f(x)$ locally using a Taylor series

$$f(x+\delta x) = f(x) + \delta x f'(x) + \frac{\delta x^2}{2} f''(x) + \text{h.o.t}$$

- Find the δx which minimizes this local quadratic approximation

$$f'(x+\delta x) = f'(x) + \delta x f''(x) = 0$$

- and rearranging

$$\delta x = -\frac{f'(x)}{f''(x)}$$

- Update for x

$$x_{n+1} = x_n - \frac{f'(x_n)}{f''(x_n)}$$

Recall from lecture 1: Taylor expansion in 2D

A function may be approximated locally by its Taylor series expansion about a point $\mathbf{x}_0$

$$f(\mathbf{x}_0 + \boldsymbol{\delta}\mathbf{x}) \approx f(\mathbf{x}_0) + \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right) \begin{pmatrix} \delta x \\ \delta y \end{pmatrix} + \frac{1}{2} (\delta x, \delta y) \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} \begin{pmatrix} \delta x \\ \delta y \end{pmatrix} + \text{h.o.t}$$

The expansion to second order is a quadratic function

$$f(\mathbf{x}_0 + \boldsymbol{\delta}\mathbf{x}) = a + \mathbf{g}^\top \boldsymbol{\delta}\mathbf{x} + \frac{1}{2} \boldsymbol{\delta}\mathbf{x}^\top \mathtt{H}\ \boldsymbol{\delta}\mathbf{x}$$

Newton's method in ND

Expand $f(\mathbf{x})$ by its Taylor series about the point $\mathbf{x}_n$

$$f(\mathbf{x}_n + \boldsymbol{\delta}\mathbf{x}) \approx f(\mathbf{x}_n) + \mathbf{g}_n^\top \boldsymbol{\delta}\mathbf{x} + \frac{1}{2}\boldsymbol{\delta}\mathbf{x}^\top \mathtt{H}_n \, \boldsymbol{\delta}\mathbf{x}$$

where the gradient is the vector

$$\mathbf{g}_n = \nabla f(\mathbf{x}_n) = \left[\frac{\partial f}{\partial x_1}, \ldots, \frac{\partial f}{\partial x_N}\right]^\top$$

and the Hessian is the symmetric matrix

$$\mathtt{H}_n = \mathtt{H}(\mathbf{x}_n) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_N} \\ \vdots & \ddots & \\ \frac{\partial^2 f}{\partial x_1 \partial x_N} & & \frac{\partial^2 f}{\partial x_N^2} \end{bmatrix}$$

For a minimum we require that $\nabla f(\mathbf{x}) = \mathbf{0}$, and so

$$\nabla f(\mathbf{x}) = \mathbf{g}_n + \mathtt{H}_n \boldsymbol{\delta}\mathbf{x} = \mathbf{0}$$

with solution $\boldsymbol{\delta}\mathbf{x} = -\mathtt{H}_n^{-1}\mathbf{g}_n$. This gives the iterative update

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \mathtt{H}_n^{-1}\mathbf{g}_n$$

Assume that H is positive definite (all eigenvalues greater than zero)

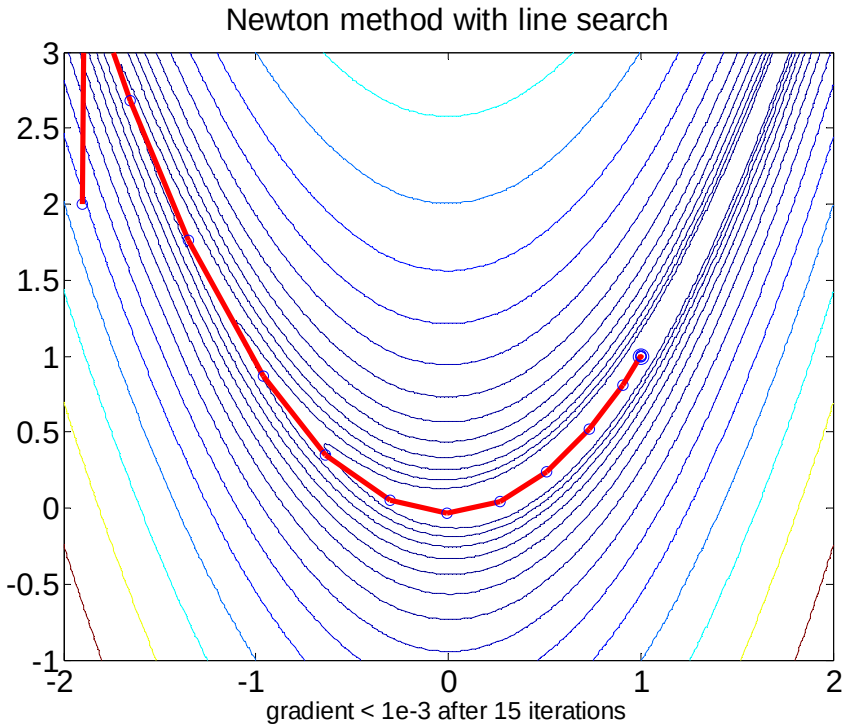
$$\begin{aligned} \mathbf{x}_{n+1} &= \mathbf{x}_n + \boldsymbol{\delta}\mathbf{x} \\ &= \mathbf{x}_n - \mathtt{H}_n^{-1}\mathbf{g}_n \end{aligned}$$

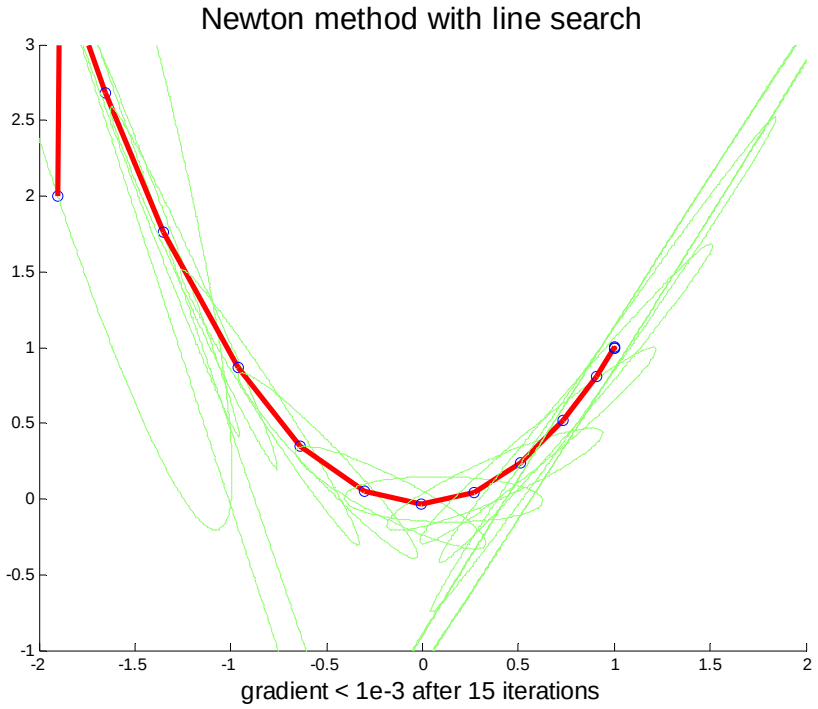
- If $f(\mathbf{x})$ is quadratic, then the solution is found in one step.
- The method has quadratic convergence (as in the 1D case).
- The solution $\boldsymbol{\delta}\mathbf{x} = -\mathtt{H}_n^{-1}\mathbf{g}_n$ is guaranteed to be a downhill direction (provided that $\mathtt{H}$ is positive definite)
- For numerical reasons the inverse is not actually computed, instead $\boldsymbol{\delta}\mathbf{x}$ is computed as the solution of $\mathtt{H}\,\boldsymbol{\delta}\mathbf{x} = -\mathbf{g}_n$.
- Rather than jump straight to $\mathbf{x}_n - \mathtt{H}_n^{-1}\mathbf{g}_n$, it is better to perform a line search which ensures global convergence

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \alpha_n \mathtt{H}_n^{-1}\mathbf{g}_n$$

- If $\mathtt{H} = \mathtt{I}$ then this reduces to steepest descent.

Newton's method - example





ellipses show successive quadratic approximations

- The algorithm converges in only 15 iterations compared to hundreds for steepest descent.
- However, the method requires computing the Hessian matrix at each iteration – this is not always feasible

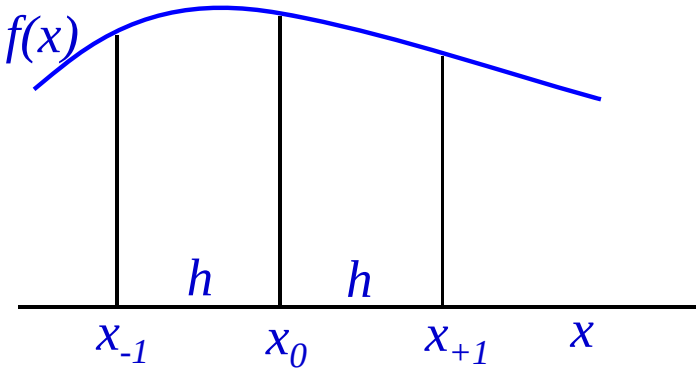
Quasi-Newton methods

- If the problem size is large and the Hessian matrix is dense then it may be infeasible/inconvenient to compute it directly.

- Quasi-Newton methods avoid this problem by keeping a "rolling estimate" of $\mathtt{H}(\mathbf{x})$, updated at each iteration using new gradient information.

- Common schemes are due to Broyden, Fletcher, Goldfarb and Shanno (BFGS), and also Davidson, Fletcher and Powell (DFP).

e.g. in 1D



First derivatives

$$f'(x_0 + \frac{h}{2}) = \frac{f_1 - f_0}{h} \quad \text{and} \quad f'(x_0 - \frac{h}{2}) = \frac{f_0 - f_{-1}}{h}$$

second derivative

$$f''(x_0) = \frac{\frac{f_1 - f_0}{h} - \frac{f_0 - f_{-1}}{h}}{h} = \frac{f_1 - 2f_0 + f_{-1}}{h^2}$$

For $\mathtt{H}_{n+1}$ build an approximation from $\mathtt{H}_n, \mathbf{g}_n, \mathbf{g}_{n+1}, \mathbf{x}_n, \mathbf{x}_{n+1}$

Quasi-Newton: BFGS

- Set $\mathtt{H}_0 = \mathtt{I}$.

- Update according to

$$\mathtt{H}_{n+1} = \mathtt{H}_n + \frac{\mathbf{q}_n \mathbf{q}_n^\top}{\mathbf{q}_n^\top \mathbf{s}_n} - \frac{(\mathtt{H}_n \mathbf{s}_n)(\mathtt{H}_n \mathbf{s}_n)^\top}{\mathbf{s}_n^\top \mathtt{H}_n \mathbf{s}_n}$$

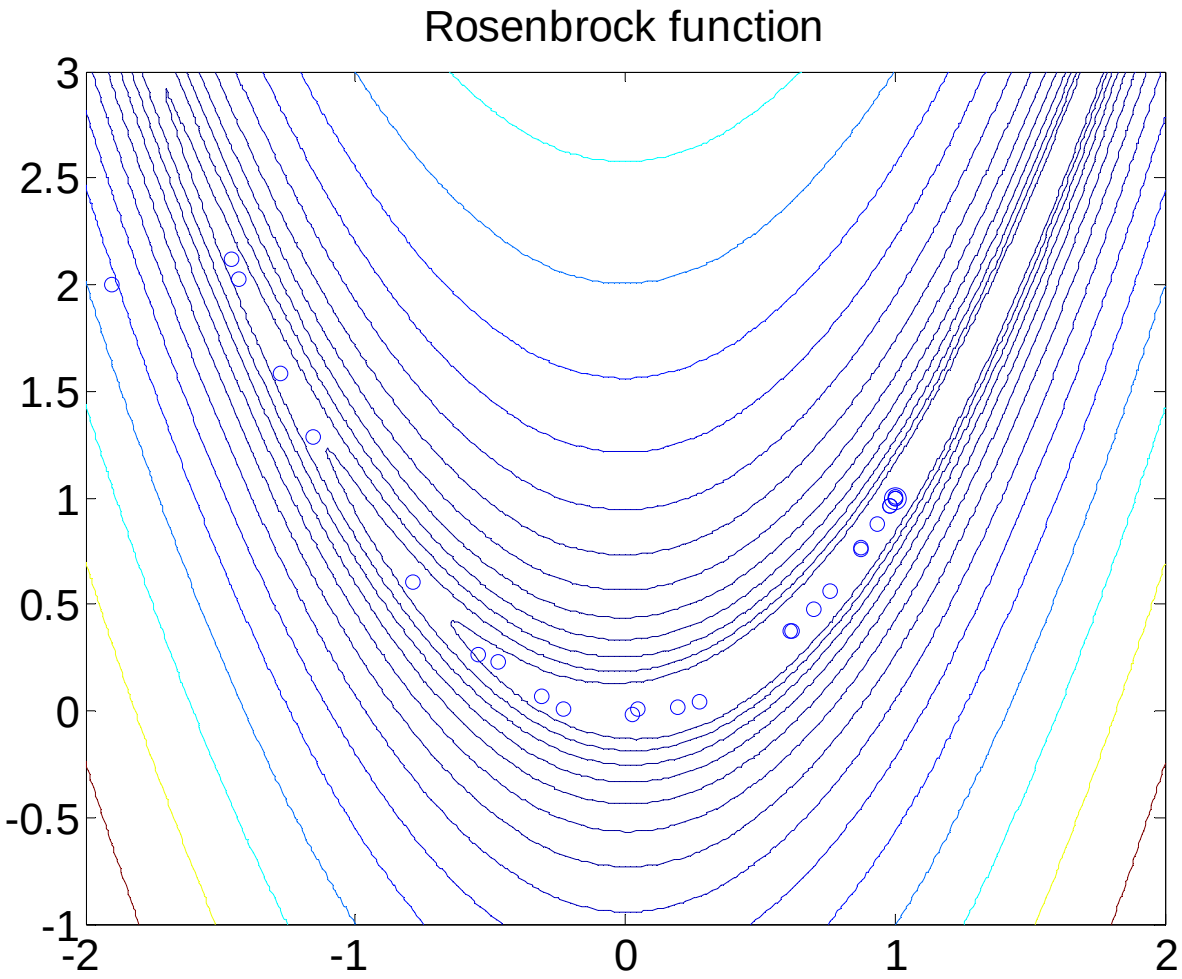
where

$$\begin{aligned} \mathbf{s}_n &= \mathbf{x}_{n+1} - \mathbf{x}_n \\ \mathbf{q}_n &= \mathbf{g}_{n+1} - \mathbf{g}_n \end{aligned}$$

- The matrix itself is not stored, but rather represented compactly by a few stored vectors.

- The estimate $\mathtt{H}_{n+1}$ is used to form a local quadratic approximation as before.

Example



- The method converges in 25 iterations, compared to 15 for the full-Newton method

- In Matlab the optimization function ‘fminunc’ uses a BFGS quasi-Newton method for medium scale optimization problems

Matlab – fminunc

```
>> f='100*(x(2)-x(1)^2)^2+(1-x(1))^2';

>> GRAD='[100*(4*x(1)^3-4*x(1)*x(2))+2*x(1)-2;  100*(2*x(2)-2*x(1)^2) ]';
```

Choose options for BFGS quasi-Newton

```
>> OPTIONS=optimset('LargeScale','off', 'HessUpdate','bfgs' );
>> OPTIONS = optimset(OPTIONS,'gradobj','on');
```

Start point

```
>> x = [-1.9; 2];

>> [x,fval] = fminunc({f,GRAD},x,OPTIONS);
```

This produces

x = 0.9998, 0.9996 fval = 3.4306e-008

Non-linear least squares

- It is **very** common in applications for a cost function $f(\mathbf{x})$ to be the sum of a large number of squared residuals

$$f(\mathbf{x}) = \sum_{i=1}^{M} r_i^2$$

- If each residual depends **non-linearly** on the parameters $\mathbf{x}$ then the minimization of $f(\mathbf{x})$ is a non-linear least squares problem.

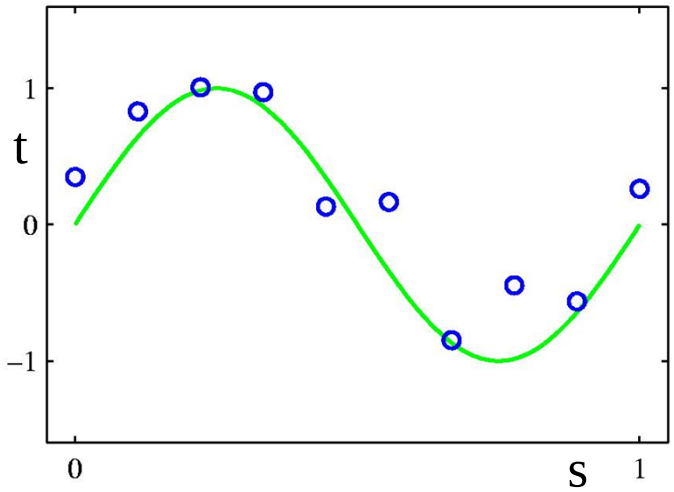
- Examples arise in non-linear regression (fitting) of data

Linear least squares reminder

The goal is to fit a smooth curve to measured data points $\{s_i, t_i\}$ by minimizing the cost

$$f(\mathbf{x}) = \sum_{i=1} r_i^2 = \sum_{i=1} (y(s_i, \mathbf{x}) - t_i)^2$$

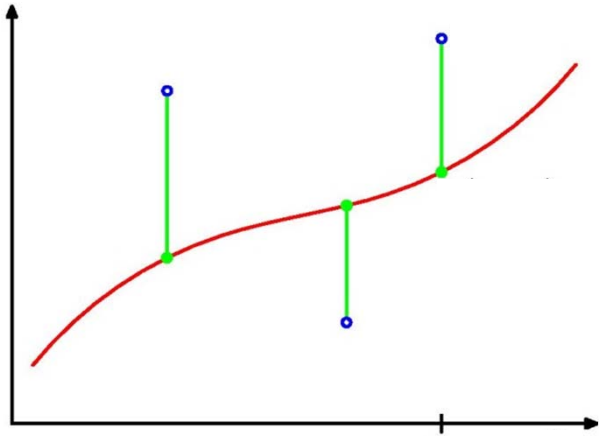
target value



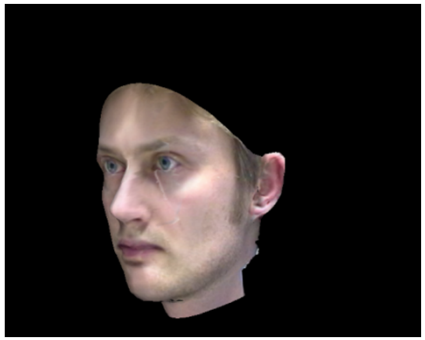
For example, the regression function $y(s_i, \mathbf{x})$ might be polynomial

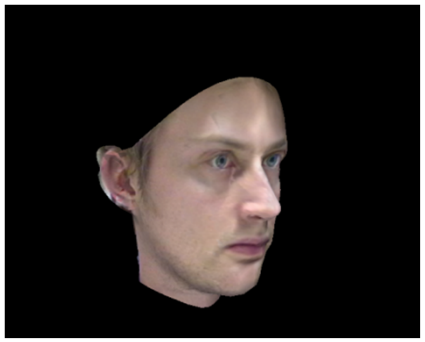
$$y(s, \mathbf{x}) = x_0 + x_1 s + x_2 s^2 + \ldots$$

In this case the function is linear in the parameter $\mathbf{x}$ and there is a closed form solution. In general there will not be a closed form solution for non-linear functions $y(s, \mathbf{x})$.



Non-linear least squares example: aligning a 3D model to an image





Input:

3D textured face model, camera model, image $I(x, y)$.

Task:

Determine the 3D rotation and 3D translation that minimizes the error between image $I(x, y)$ and the projected 3D model

Cost function

$$f(\mathtt{R}, \mathbf{T}) = \sum_{x,y}^{M} |\hat{I}_{\mathtt{R},\mathbf{T}}(x, y) - I(x, y)|^2$$

Transformation parameters:

- 3D rotation matrix $\mathtt{R}$
- translation 3-vector $\mathbf{T} = (T_x, T_y, T_z)^\top$

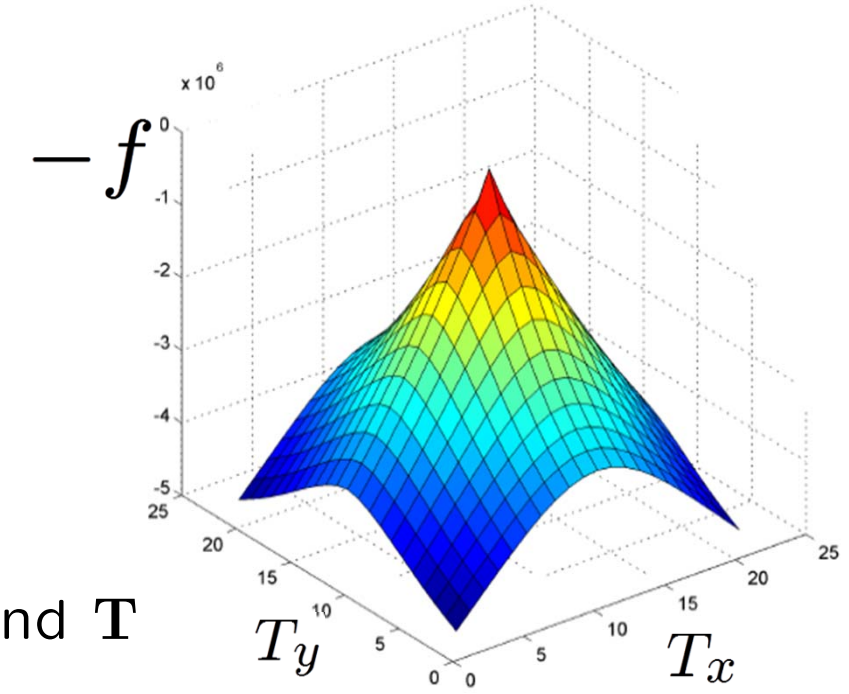


Image generation:

- rotate and translate 3D model by $\mathtt{R}$ and $\mathbf{T}$
- project to generate image $\hat{I}_{\mathtt{R},\mathbf{T}}(x, y)$

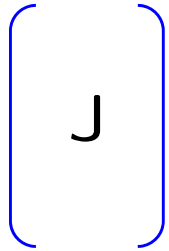
Non-linear least squares

$$f(\mathbf{x}) = \sum_{i=1}^{M} r_i^2 = \|\mathbf{r}\|^2$$

The $M \times N$ **Jacobian** of the vector of residuals $\mathbf{r}$ is defined as

assume M > N

$$\mathrm{J}(\mathbf{x}) = \begin{pmatrix} \frac{\partial r_1}{\partial x_1} & \cdots & \frac{\partial r_1}{\partial x_N} \\ \vdots & \ddots & \\ \frac{\partial r_M}{\partial x_1} & & \frac{\partial r_M}{\partial x_N} \end{pmatrix}$$

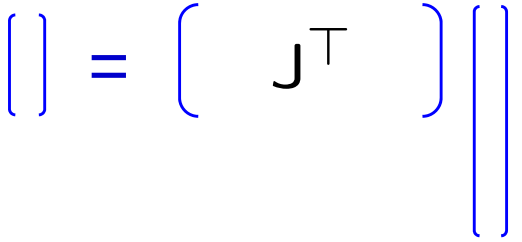


Consider

$$\frac{\partial}{\partial x_k} \sum_i r_i^2 = \sum_i 2 r_i \frac{\partial r_i}{\partial x_k}$$

Hence

$$\nabla f(\mathbf{x}) = 2\mathrm{J}^\top \mathbf{r}$$



For the Hessian we require

$$\begin{aligned}\frac{\partial^2}{\partial x_l \partial x_k}\sum_i r_i^2 &= 2\frac{\partial}{\partial x_l}\sum_i r_i \frac{\partial r_i}{\partial x_k} \\ &= 2\sum_i \frac{\partial r_i}{\partial x_k}\frac{\partial r_i}{\partial x_l} + 2\sum_i r_i \frac{\partial^2 r_i}{\partial x_k \partial x_l}\end{aligned}$$

Hence

$$\mathtt{H}(\mathbf{x}) = \quad 2\mathtt{J}^\top\mathtt{J} \quad + \quad 2\sum_{i=1}^{M} r_i \mathtt{R}_i$$

$$\begin{pmatrix} \mathtt{J}^\top \end{pmatrix}\begin{pmatrix} \mathtt{J} \\ \\ \end{pmatrix} \qquad \begin{pmatrix} \mathtt{R_i} \end{pmatrix}$$

- Note that the second-order term in the Hessian $\mathtt{H}(\mathbf{x})$ is multiplied by the residuals r_i.

- In most problems, the residuals will typically be small.

- Also, at the minimum, the residuals will typically be distributed with mean $= 0$.

- For these reasons, the second-order term is often ignored, giving the Gauss-Newton approximation to the Hessian :

$$\mathtt{H}(\mathbf{x}) = 2\mathtt{J}^\top \mathtt{J}$$

- Hence, explicit computation of the full Hessian can again be avoided.

Example – Gauss-Newton

The minimization of the Rosenbrock function

$$f(x, y) = 100(y - x^2)^2 + (1 - x)^2$$

can be written as a least-squares problem with residual vector

$$\mathbf{r} = \begin{bmatrix} 10(y - x^2) \\ (1 - x) \end{bmatrix}$$

$$\mathtt{J}(\mathbf{x}) = \begin{pmatrix} \frac{\partial r_1}{\partial x} & \frac{\partial r_1}{\partial y} \\ \frac{\partial r_2}{\partial x} & \frac{\partial r_2}{\partial y} \end{pmatrix} = \begin{pmatrix} -20x & 10 \\ -1 & 0 \end{pmatrix}$$

The true Hessian is

$$\mathtt{H}(\mathbf{x}) = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 1200x^2 - 400y + 2 & -400x \\ -400x & 200 \end{bmatrix}$$

The Gauss-Newton approximation of the Hessian is

$$2\mathtt{J}^\top \mathtt{J} = 2 \begin{bmatrix} -20x & -1 \\ 10 & 0 \end{bmatrix} \begin{bmatrix} -20x & 10 \\ -1 & 0 \end{bmatrix} = \begin{bmatrix} 800x^2 + 2 & -400x \\ -400x & 200 \end{bmatrix}$$

Summary: Gauss-Newton optimization

For a cost function $f(\mathbf{x})$ that is a sum of squared residuals

$$f(\mathbf{x}) = \sum_{i=1} r_i^2$$

The Hessian can be approximated as

$$\mathtt{H}(\mathbf{x}) = 2\mathtt{J}^\top \mathtt{J}$$

and the gradient is given by

$$\nabla f(\mathbf{x}) = 2\mathtt{J}^\top \mathbf{r}$$

So, the Newton update step

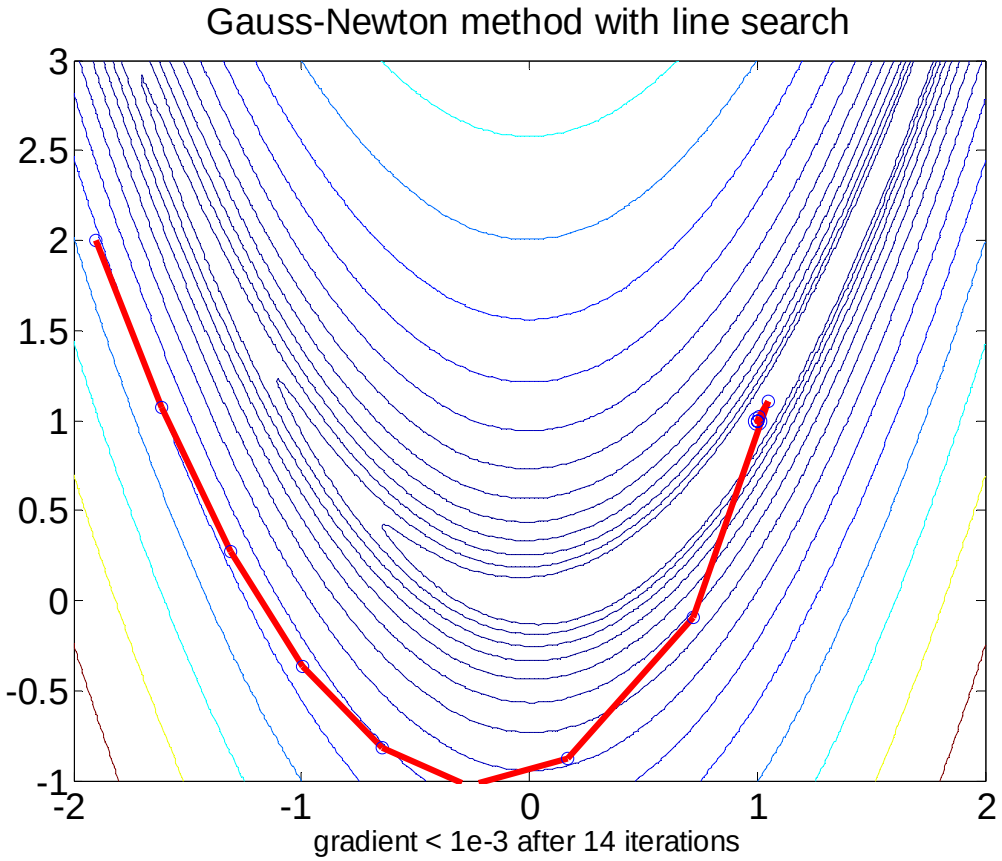
$$\begin{aligned} \mathbf{x}_{n+1} &= \mathbf{x}_n + \boldsymbol{\delta}\mathbf{x} \\ &= \mathbf{x}_n - \mathtt{H}_n^{-1}\mathbf{g}_n \end{aligned}$$

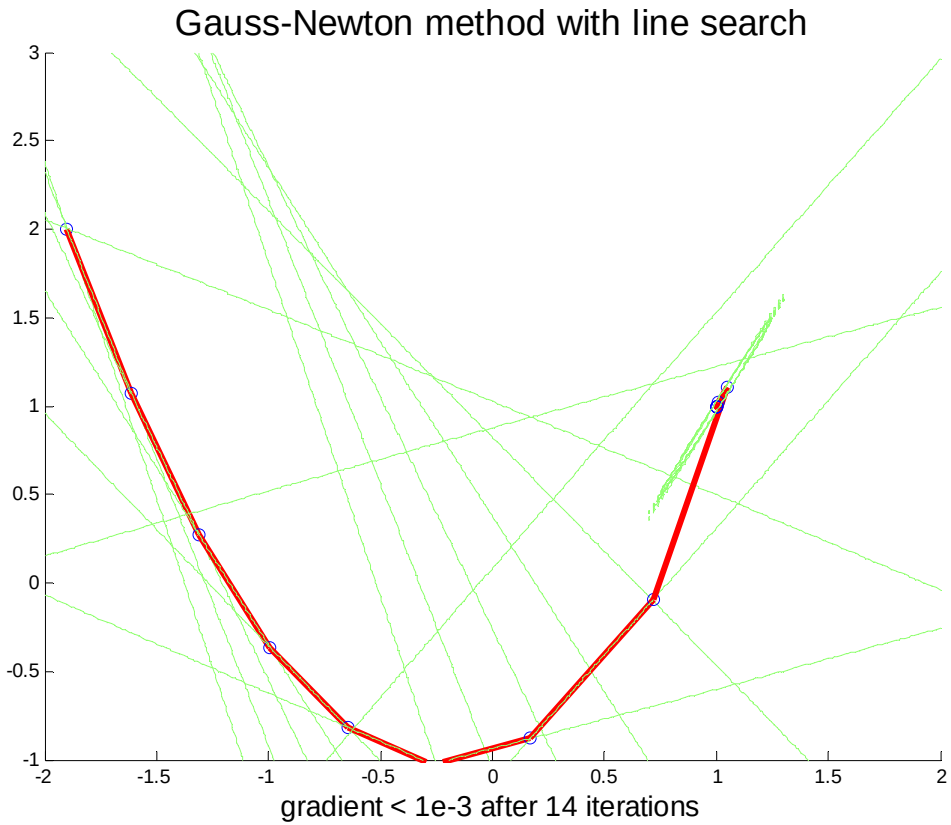
computed as $\mathtt{H}\,\boldsymbol{\delta}\mathbf{x} = -\mathbf{g}_n$, becomes

$$\mathtt{J}^\top \mathtt{J}\,\boldsymbol{\delta}\mathbf{x} = -\mathtt{J}^\top \mathbf{r}$$

These are called the normal equations.

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \alpha_n \mathbf{H}_n^{-1} \mathbf{g}_n \quad \text{with} \quad \mathbf{H}_n(\mathbf{x}) = 2\mathbf{J}_n^\top \mathbf{J}_n$$

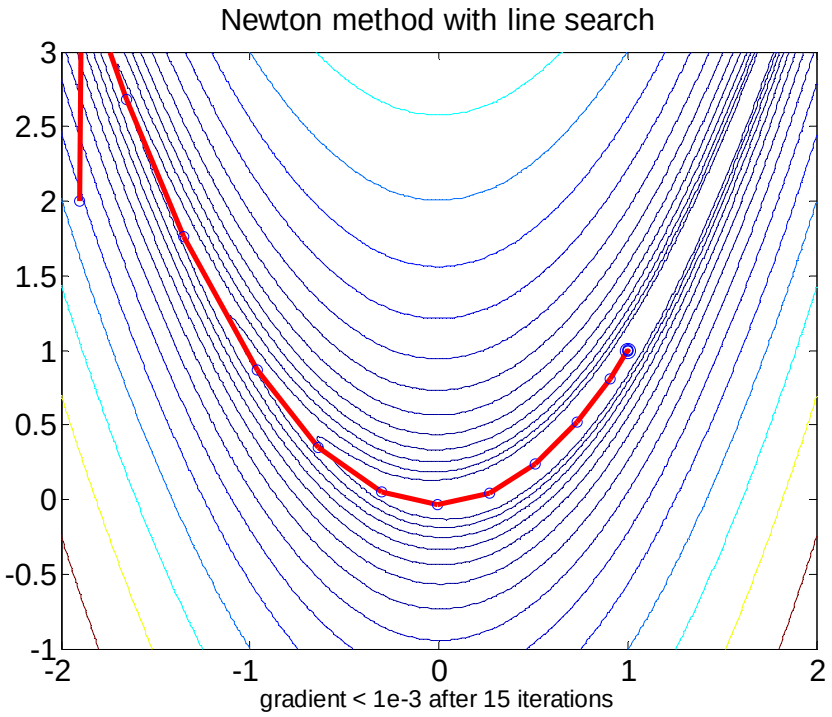




- minimization with the Gauss-Newton approximation with line search takes only 14 iterations

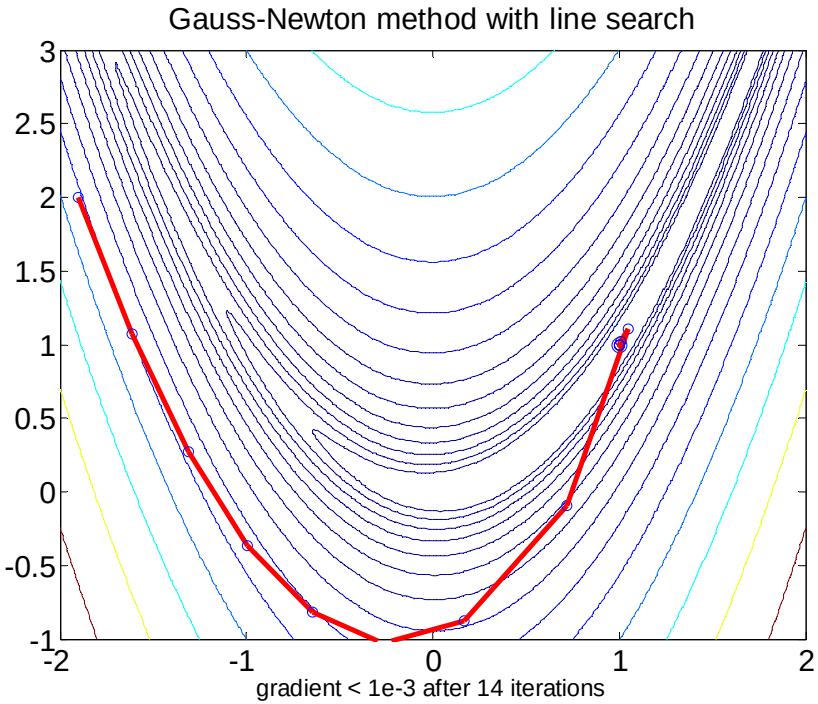
Comparison

Newton



- requires computing Hessian (i.e. n^2 second derivatives)
- exact solution if quadratic

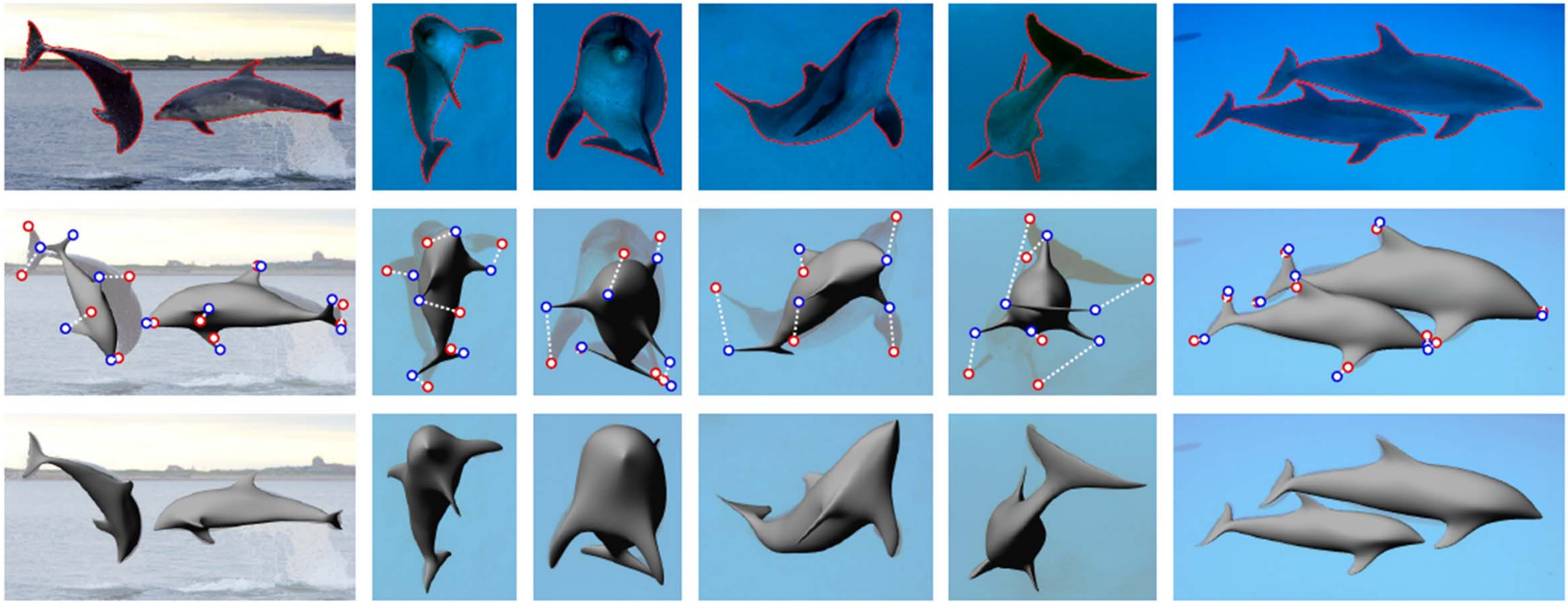
Gauss-Newton



- approximates Hessian by Jacobian product
- requires only n first derivatives

Application: Building 3D morphable models from 2D images

Optimize over point correspondences for 3D and morphing parameters using non-linear least squares



What Shape are Dolphins? Building 3DMorphable Models from 2D Images, Cashman and Fitzgibbon, PAMI 2012

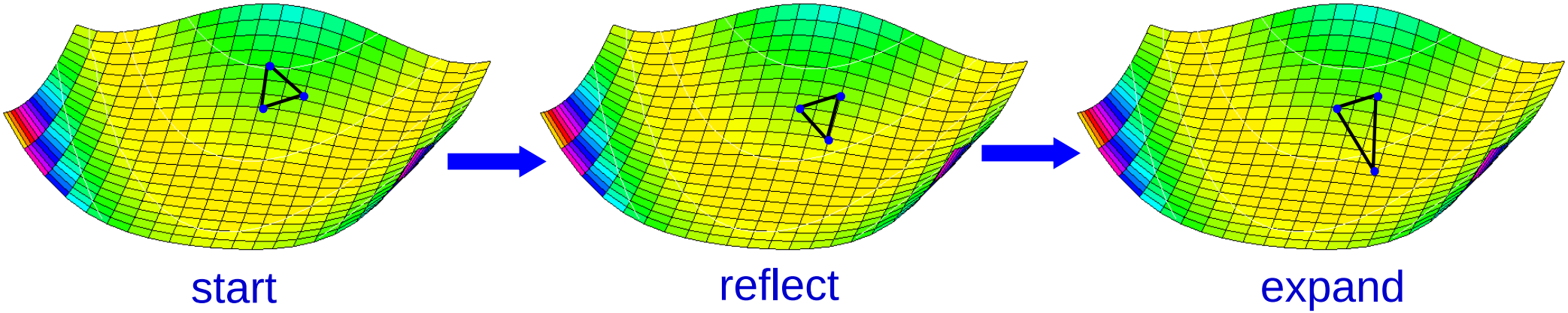
Properties of methods

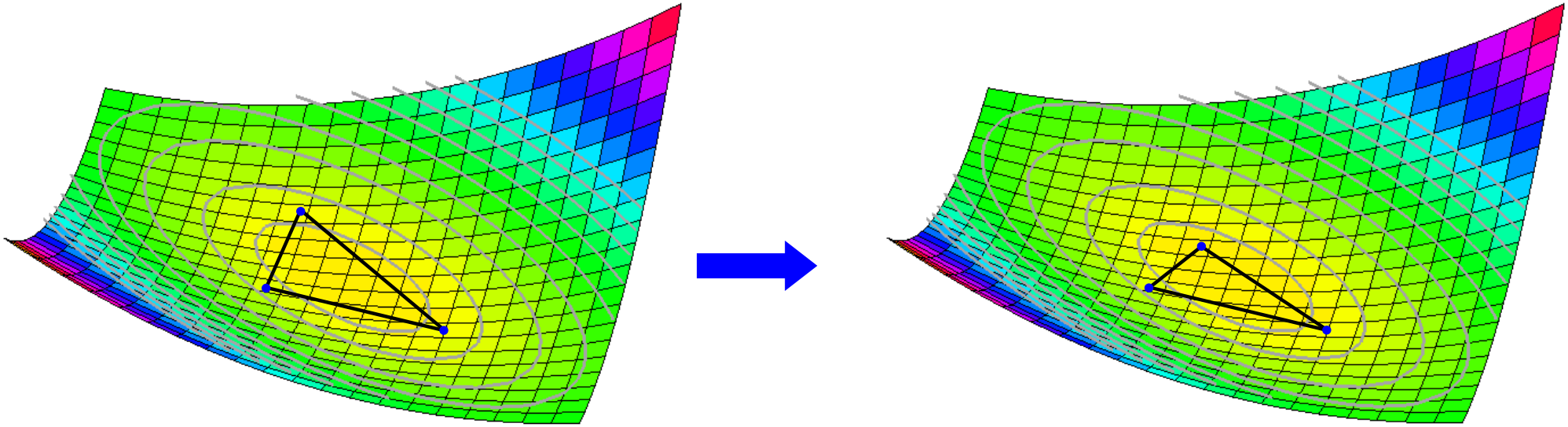
- **Gradient descent**
  - will zig-zag – each new increment is perpendicular to previous.
  - Requires 1D search
  - Slow to converge.
- **Newton's method**
  - requires computation of Hessian.
  - Can converge to maximum or saddle as well as minimum.
  - Can be unstable.
- **Gauss-Newton**
  - Is a downhill method, so will not converge to maximum or saddle.
  - Can be unstable, thus preferably needs line search.

The downhill simplex (amoeba) algorithm

The downhill simplex (amoeba) algorithm

- Due to Nelder and Mead (1965)
- A *direct* method: only uses function evaluations (no derivatives)
- a simplex is the polytope in *N* dimensions with *N+1* vertices, e.g.
  - 2D: triangle
  - 3D: tetrahedron
- basic idea: move by reflections, expansions or contractions




contract

One iteration of the simplex algorithm

- Reorder the points so that $f(\mathbf{x}_{n+1}) > f(\mathbf{x}_2) > f(\mathbf{x}_1)$ (i.e. $\mathbf{x}_{n+1}$ is the worst point).

- Generate a trial point $\mathbf{x}_r$ by *reflection*

$$\mathbf{x}_r = \bar{\mathbf{x}} + \alpha(\bar{\mathbf{x}} - \mathbf{x}_{n+1})$$

where $\bar{\mathbf{x}} = \left(\sum_i \mathbf{x}_i\right)/(N+1)$ is the centroid and $\alpha > 0$. Compute $f(\mathbf{x}_r)$, and there are then 3 possibilities:

1. $f(\mathbf{x}_1) < f(\mathbf{x}_r) < f(\mathbf{x}_n)$ (i.e. $\mathbf{x}_r$ is neither the new best or worst point), replace $\mathbf{x}_{n+1}$ by $\mathbf{x}_r$.

2. $f(\mathbf{x}_r) < f(\mathbf{x}_1)$ (i.e. $\mathbf{x}_r$ is the new best point), then assume direction of reflection is good and generate a new point by *expansion*

$$\mathbf{x}_e = \mathbf{x}_r + \beta(\mathbf{x}_r - \bar{\mathbf{x}})$$

where $\beta > 0$. If $f(\mathbf{x}_e) < f(\mathbf{x}_r)$ then replace $\mathbf{x}_{n+1}$ by $\mathbf{x}_e$, otherwise, the expansion has failed, replace $\mathbf{x}_{n+1}$ by $\mathbf{x}_r$.

3. $f(\mathbf{x}_r) > f(\mathbf{x}_n)$ then assume the polytope is too large and generate a new point by *contraction*

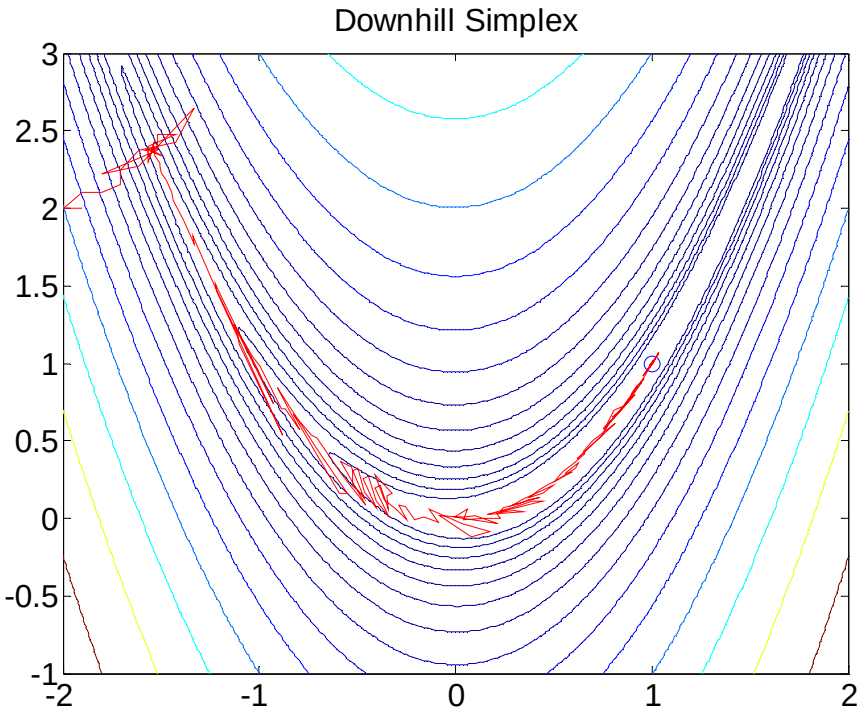
$$\mathbf{x}_c = \bar{\mathbf{x}} + \gamma(\mathbf{x}_{n+1} - \bar{\mathbf{x}})$$

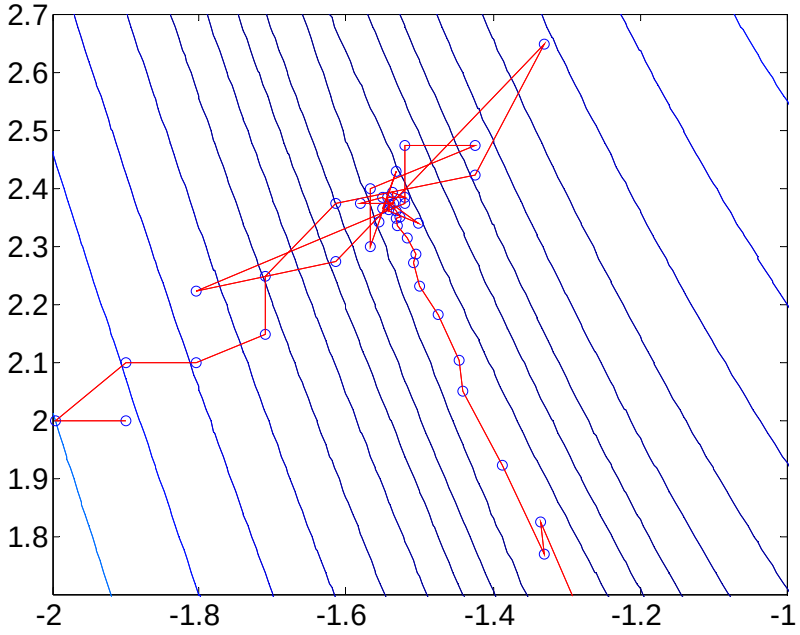
where γ $(0 < \gamma < 1)$ is the contraction coefficient. If $f(\mathbf{x}_c) < f(\mathbf{x}_{n+1})$ then the contraction has succeeded and replace $\mathbf{x}_{n+1}$ by $\mathbf{x}_c$, otherwise contract again.

Standard values are $\alpha = 1, \beta = 1, \gamma = 0.5$.

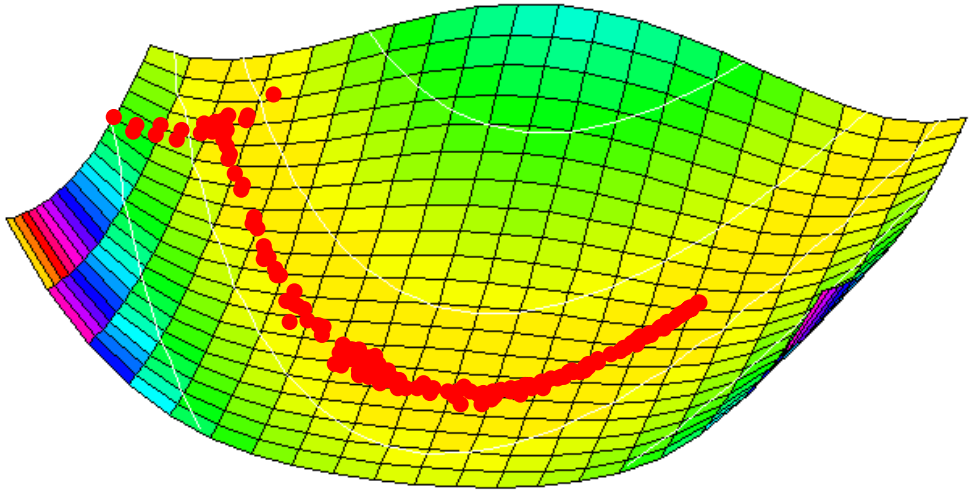
Example

Path of best vertex



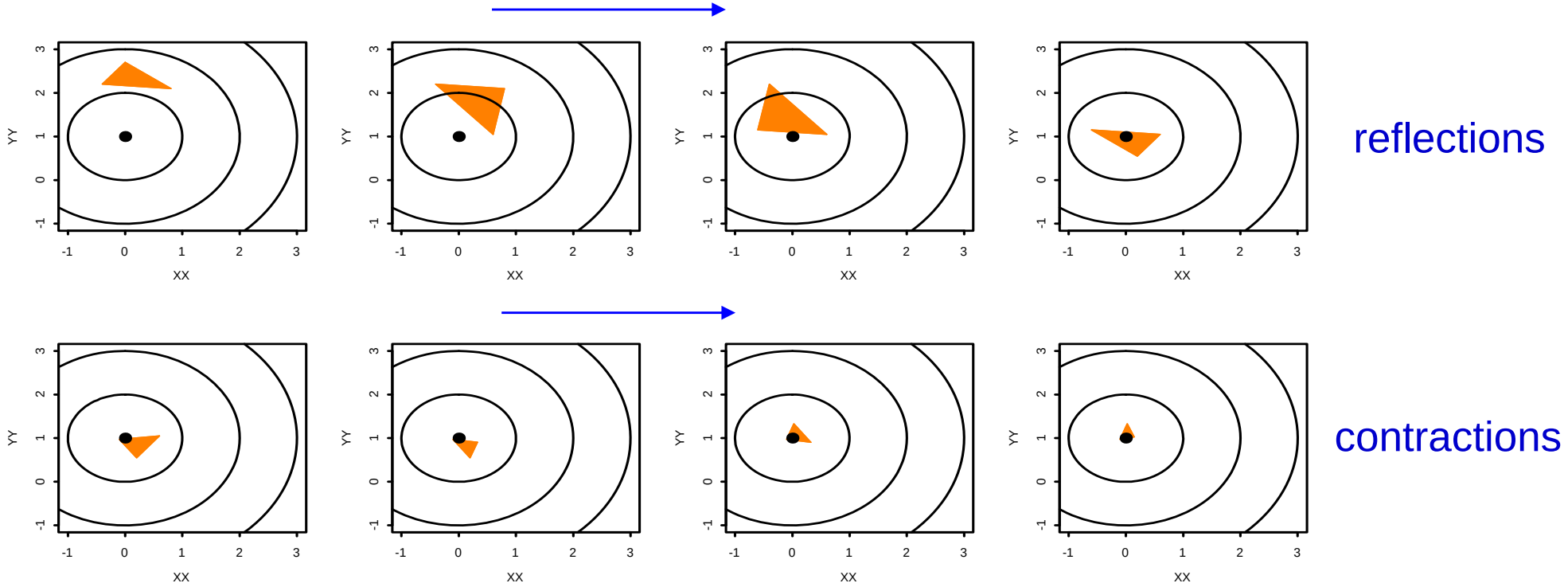


detail



Matlab fminsearch
with 200 iterations

Example 2: contraction about a minimum



Summary

- no derivatives required
- deals well with noise in the cost function
- is able to crawl out of some local minima (though, of course, can still get stuck)

Matlab – fminsearch

Nelder-Mead simplex direct search

```
>> banana = @(x)100*(x(2)-x(1)^2)^2+(1-x(1))^2;
```

Pass the function handle to fminsearch:

```
>> [x,fval] = fminsearch(banana,[-1.9, 2])
```

This produces

```
x = 1.0000  1.0000

fval =4.0686e-010
```

Google to find out more on using this function

What is next?

- Move from general and quadratic optimization problems to linear programming

- Constrained optimzation