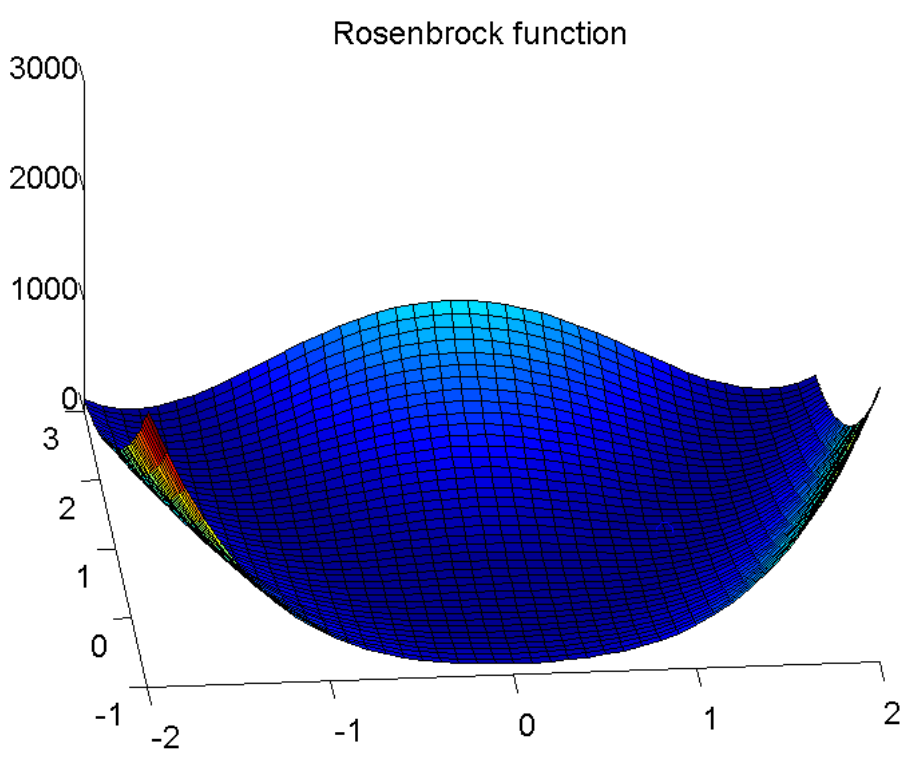
Lecture 2

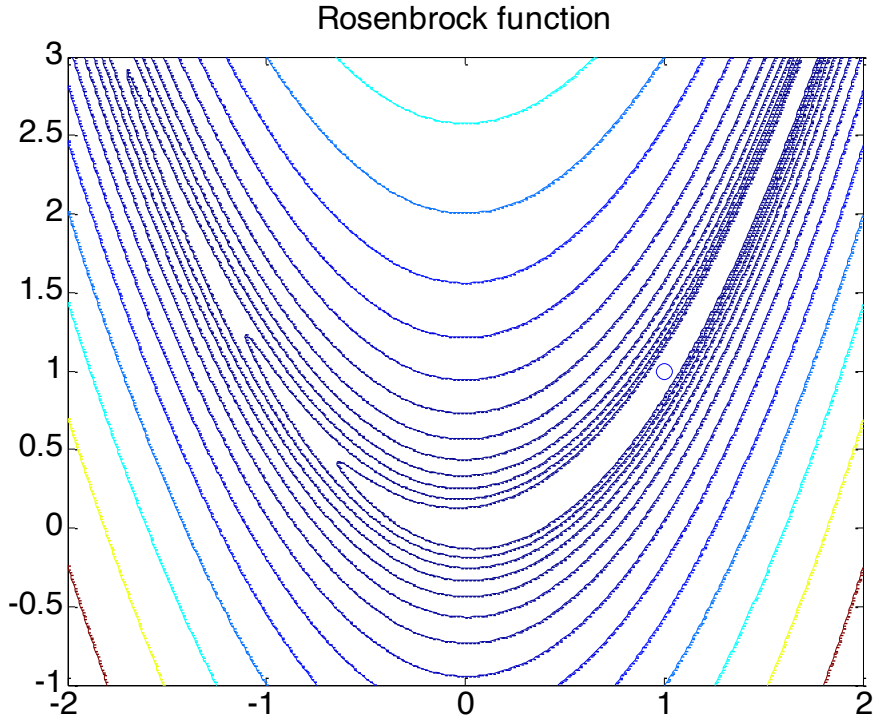
B1 Optimization - Trinity 2019 / Michaelmas 2020 - V. A. Prisacariu

- Rosenbrock's function
- Newton's method
  - Line search
- Quasi-Newton methods
- Least-Squares and Gauss-Newton methods and a few words on Levenberg-Marquardt.
- Downhill simplex (amoeba) algorithm

Rosenbrock's function

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





Minimum is at [1, 1]

An Optimization Algorithm (from lecture 1)

Start at $\mathbf{x}_0$ then repeat:

1. Compute a search direction $\mathbf{p}_k$.
2. Compute a step length α_k, such that $f(\mathbf{x}_k + \alpha_k \mathbf{p}_k) < f(\mathbf{x}_k)$.
3. Update $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{p}_k$
4. Check for convergence (termination criteria), e.g. $\nabla f \approx 0$.

Reduce optimization in N dimensions to a series of (1D) line minimizations.

Steepest descent (from lecture 1)

Basic principle is to minimize the N-dimensional function by a series of 1D line-minimizations:

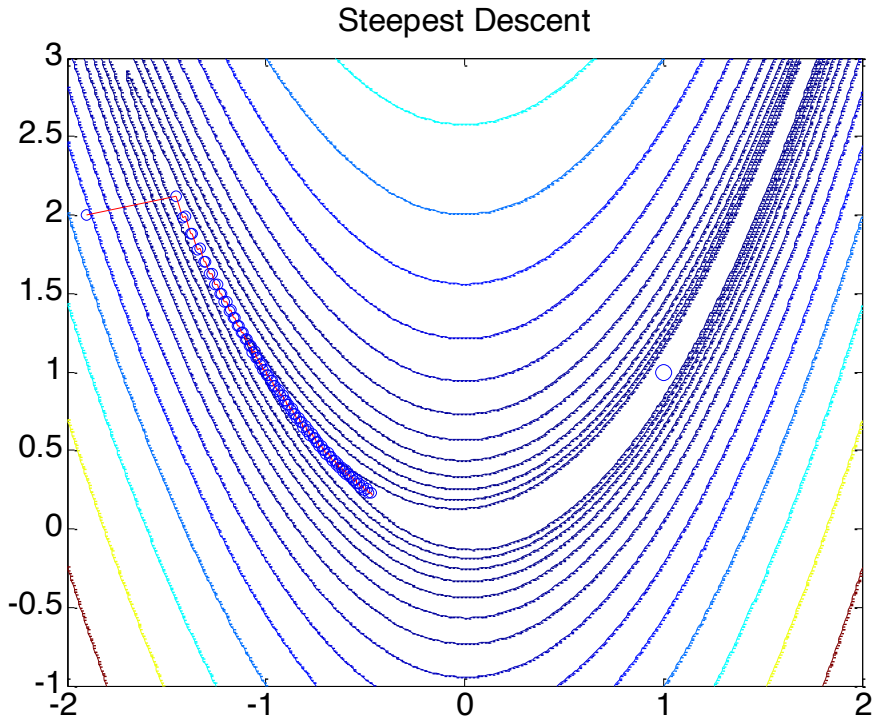
$$\mathbf{x}_{n+1} = \mathbf{x}_n + \alpha_n \mathbf{p}_n$$

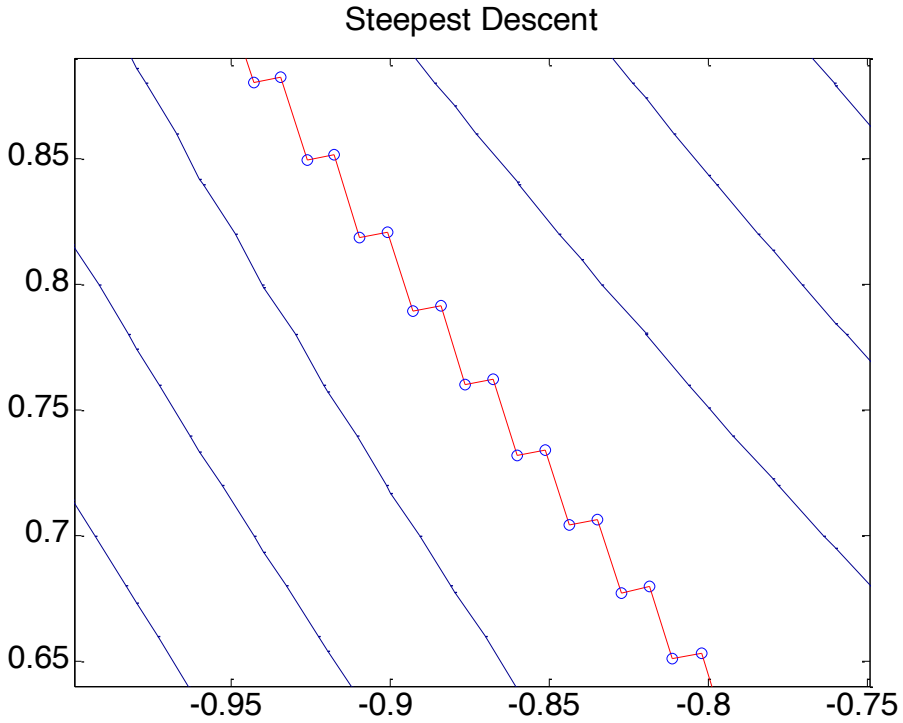
The steepest decent method choses $\mathbf{p}_n$ to be parallel to the negative gradient:

$$\mathbf{p}_n = -\nabla f(\boldsymbol{x}_{\mathrm{n}})$$

Steepest descent

The 1D line minimization must be performed using one of the earlier methods





- The zig-zag behavior is clear in the zoomed view (100 iterations);
- The algorithm crawls along the valley.

Newton's method in 1D (from lecture 1)

Fit a quadratic approx. to $f(x)$ using both gradient and curvature information at 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 such that $x + \delta x$ is a stationary point of f:

$$\frac{d}{d\delta x}\left(f(x) + \delta x f'(x) + \frac{\delta x^2}{2} f''(x) \right) = f'(x) + \delta x f''(x) = 0$$

- and rearranging:

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

- Update for x:

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

Taylor expansion in 2D (from lecture 1)

A function can be approximated locally by its Taylor series expansion about a point x_0.

$$f(x_0 + x) \approx f(x_0) + \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right)\begin{pmatrix} x \\ y \end{pmatrix} + \frac{1}{2}(x, y)\begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix}\begin{pmatrix} x \\ y \end{pmatrix} + \text{h.o.t.}$$

- This is a generalization of the 1D Taylor series:

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

- The expansion to second order is a quadratic function in $\mathbf{x}$.

$$f(\mathbf{x}) = a + \mathbf{g}^T\mathbf{x} + \frac{1}{2}\mathbf{x}^T \mathrm{H}\mathbf{x}$$

Newton's method in ND

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

$$f(\mathbf{x}_n + \delta\mathbf{x}) \approx f(\mathbf{x}_n) + \mathbf{g}_n^T \delta\mathbf{x} + \frac{1}{2}\delta\mathbf{x}^T \mathrm{H}_n \delta\mathbf{x}$$

where the gradient is the vector

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

and the Hessian is the symmetric matrix

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

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

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

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

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

Newton's method in ND

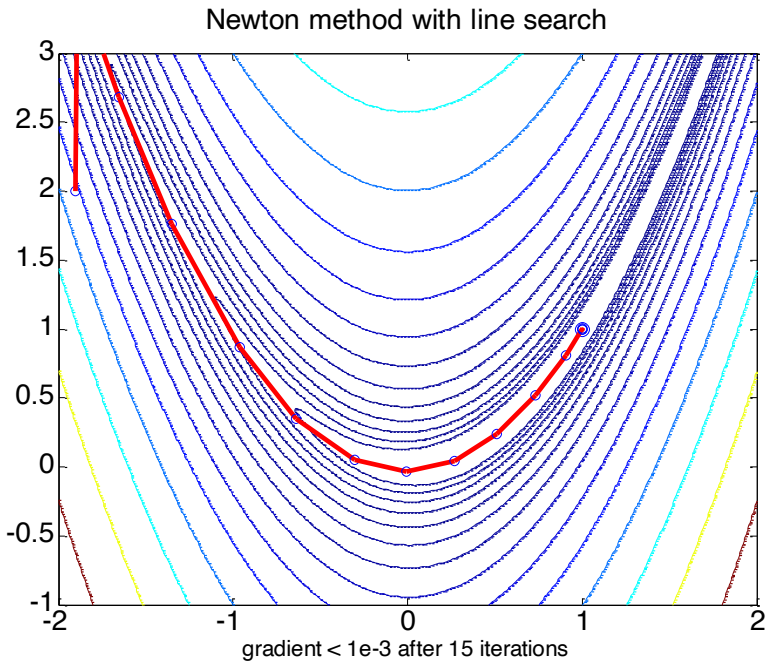
$$\mathbf{x}_{n+1} = \mathbf{x}_n + \delta\mathbf{x} = \mathbf{x}_n - \mathrm{H}_n^{-1}\mathbf{g}_n$$

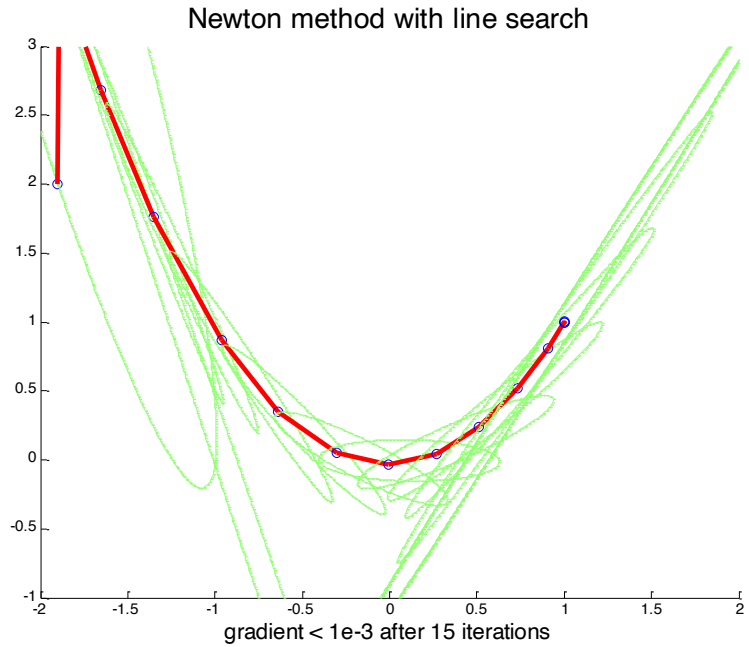
- If $f(\mathbf{x})$ is quadratic, the solution is found in one step.
- The method has quadratic convergence (as in the 1D case).
- The solution $\delta\mathbf{x} = -\mathrm{H}_n^{-1}\mathbf{g}_n$ is guaranteed to be a downhill direction (provided that H is positive definite).
- For numerical reasons,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

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

- If $\mathrm{H} = \mathrm{I}$, Newton reduces to steepest descent.

Newton's method in ND Example





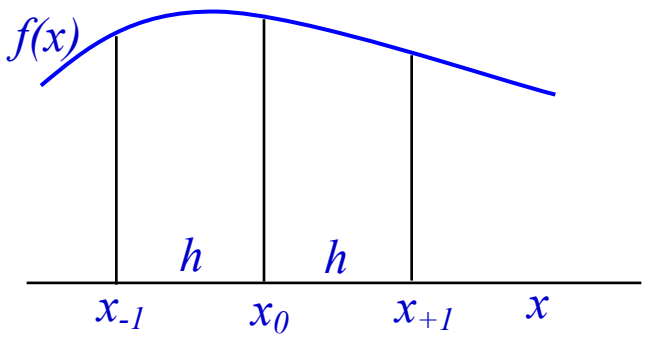
ellipses show successive quadratic approximations

- 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 in infeasible / inconvenient to compute it directly.
- Quasi-Newton method avoid this problem by keeping “rolling estimate” of $\mathrm{H}(\mathbf{x})$, updated at each iteration using new gradient information.
- Common schemes are Broyden–Fletcher–Goldfarb–Shanno (BFGS) and Davidon–Fletcher–Powell (DFP).

e.g. in 1D



First derivatives:

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

Second derivatives:

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

For H_{n+1} we can build an approximation from $\mathrm{H}_n, \mathbf{g}_n, \mathbf{g}_{n+1}, \mathbf{x}_n, \mathbf{x}_{n+1}$

Quasi-Newton BFGS

Set $\mathrm{H}_0 = \mathrm{I}$.

Update according to

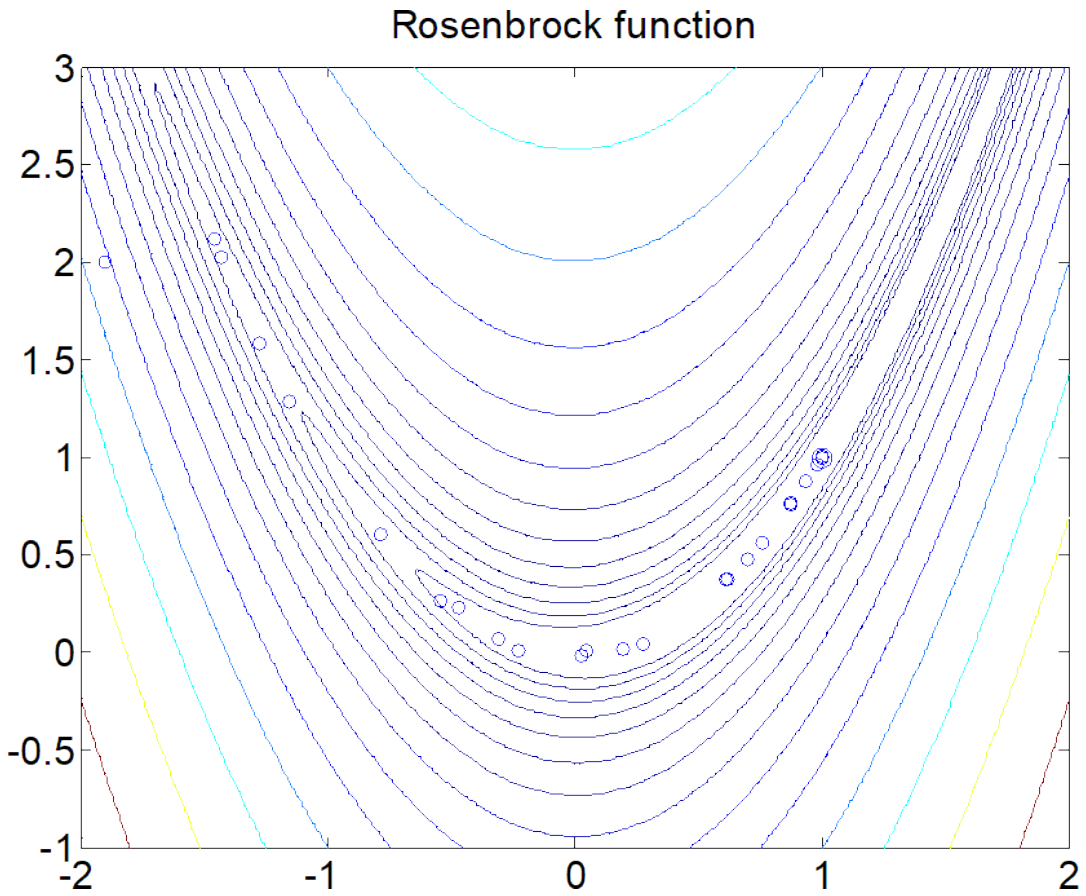
$$\mathrm{H}_{n+1} = \mathrm{H}_n + \frac{\mathbf{q}_n \mathbf{q}_n^T}{\mathbf{q}_n^T \mathbf{s}_n} - \frac{(\mathrm{H}_n \mathbf{s}_n)(\mathrm{H}_n \mathbf{s}_n)^T}{\mathbf{s}_n^T \mathrm{H}_n \mathbf{s}_n}$$

where

$$\mathbf{s}_n = \mathbf{x}_{n+1} - \mathbf{x}_n$$
$$\mathrm{q}_n = \mathbf{g}_{n+1} - \mathbf{g}_n$$

- The matrix itself is not stored, but rather represented compactly by a few stored vectors.
- The estimate H_{n+1} is used to form a local quadratic approximation as before.

Quasi-Newton BFGS 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:

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

- 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.

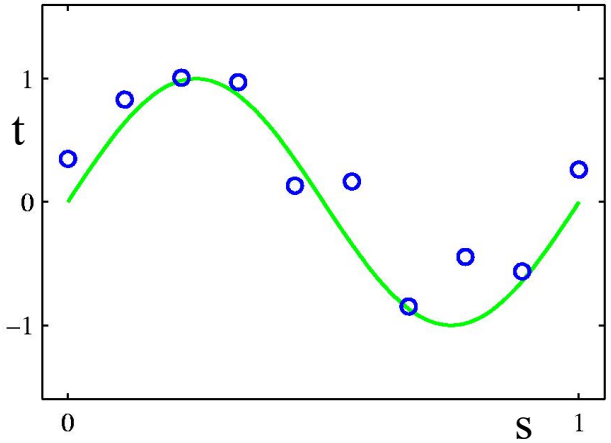
- Examples arise in non-linear regression (fitting) of data.

Linear Least Squares Reminder

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

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

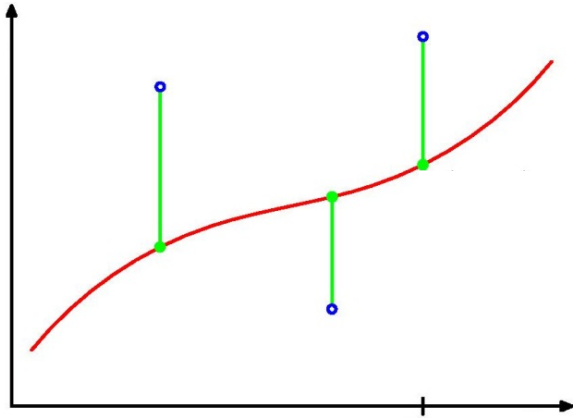
$$= \sum_{i=1} (y(s_i, \mathbf{x}) - t_i)^2 \text{ , where } t_i \text{ is the target value}$$



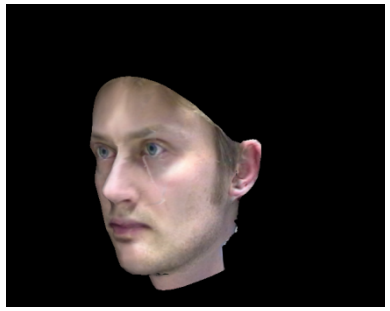
For example, the regression functions $y(s_i, \mathbf{x})$ might be the polynomial

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

In this case the function is linear in the parameter $\mathbf{x}$ and there is a closed form solution. In general there will be no closed form solution to non-linear $y(s, \mathbf{x})$.



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 the image $I(x, y)$ and the projected 3D model.

Cost Function

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

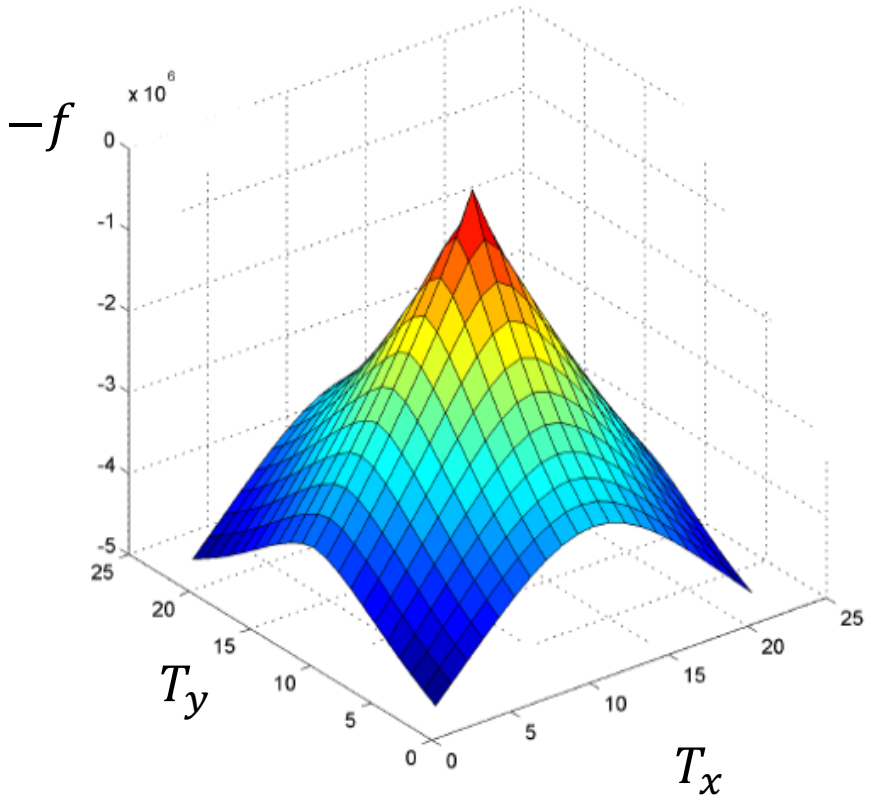
N=6, M = 10^6

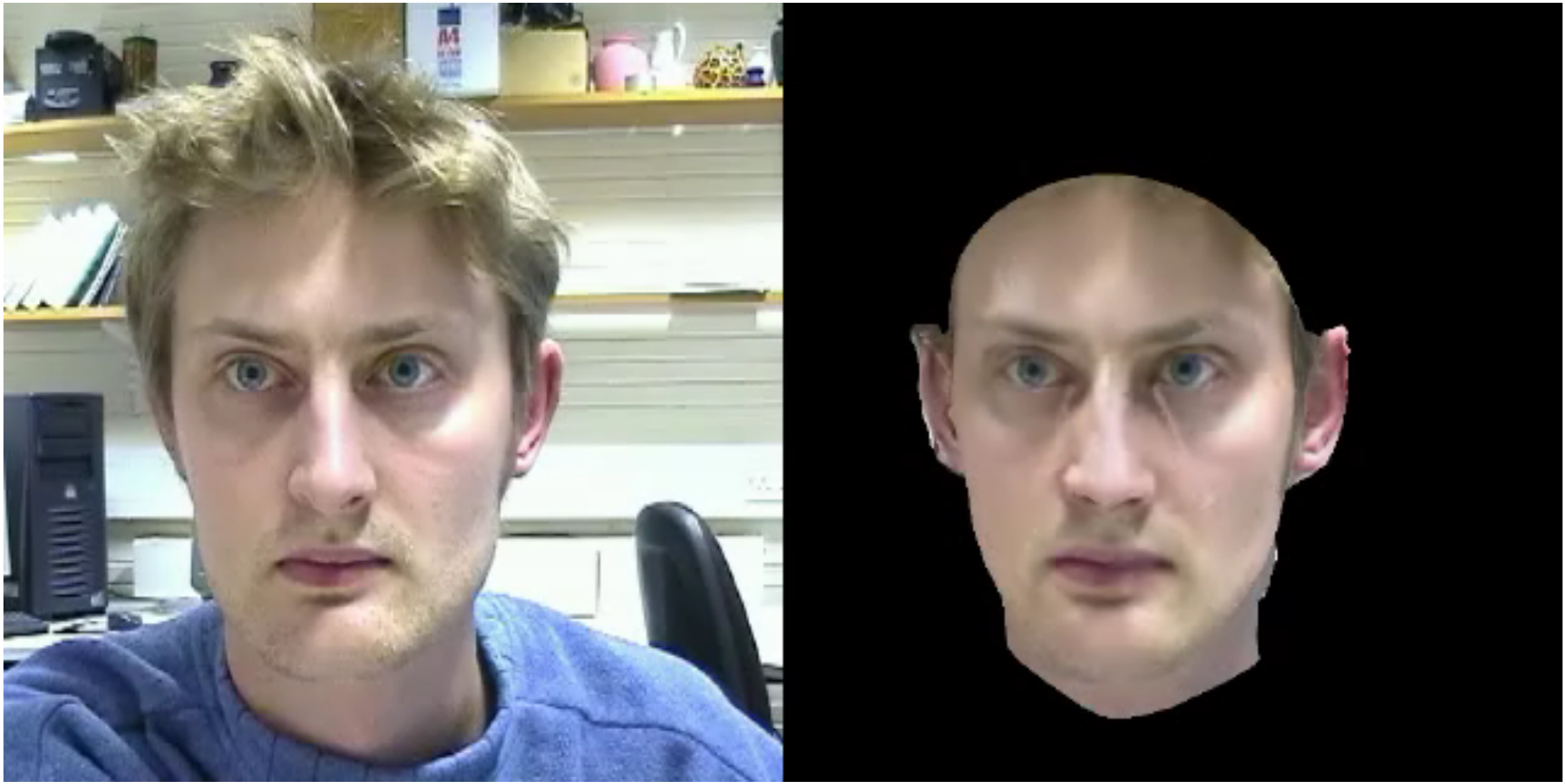
Transformation parameters:

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

Image generation:

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



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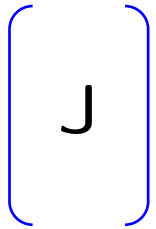
Non-Linear Least Squares

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

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

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

assume
M > N

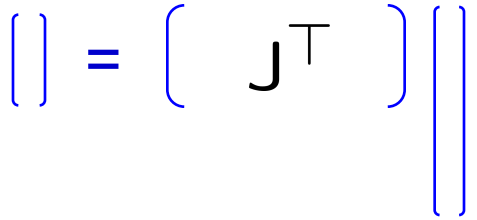


Consider

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

Hence

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



Non-Linear Least Squares

For the Hessian we require

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

Hence

$$\mathrm{H}(\mathbf{x}) = 2\mathrm{J}^T\mathrm{J} + 2 \sum_i^M r_i \mathrm{R}_i$$

R_i

$\mathrm{J}^\top$ J

Non-Linear Least Squares

Note that the second-order term in the Hessian $\mathrm{H}(\mathbf{x})$ 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 of the Hessian:

$$\mathrm{H}(\mathbf{x}) = 2\mathrm{J}^T\mathrm{J}$$

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

Gauss-Newton Example

The minimization of the Rosenbrock function.

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

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

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

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

Gauss-Newton Example

The true Hessian is:

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

The Gauss-Newton approximation of the Hessian is:

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

Gauss-Newton Summary

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

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

The Hessian can be approximated as

$$\mathrm{H}(\mathbf{x}) = 2\mathrm{J}^T\mathrm{J}$$

and the gradient is given by

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

So the Newton update step

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

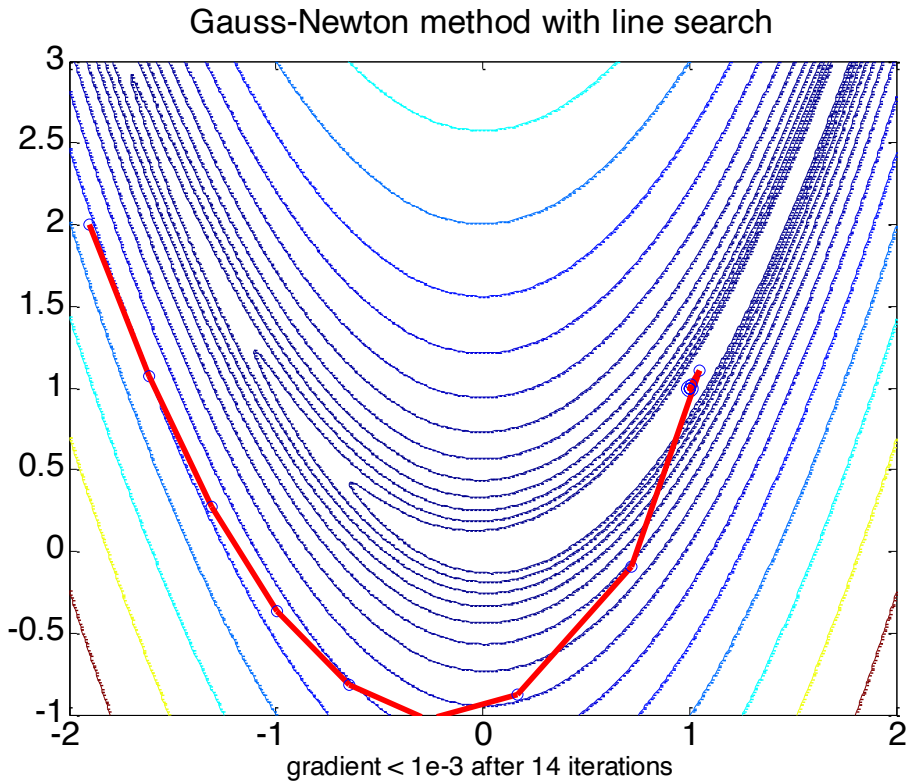
Computed as $\mathrm{H}\delta\mathbf{x} = -\mathbf{g}_n$, becomes

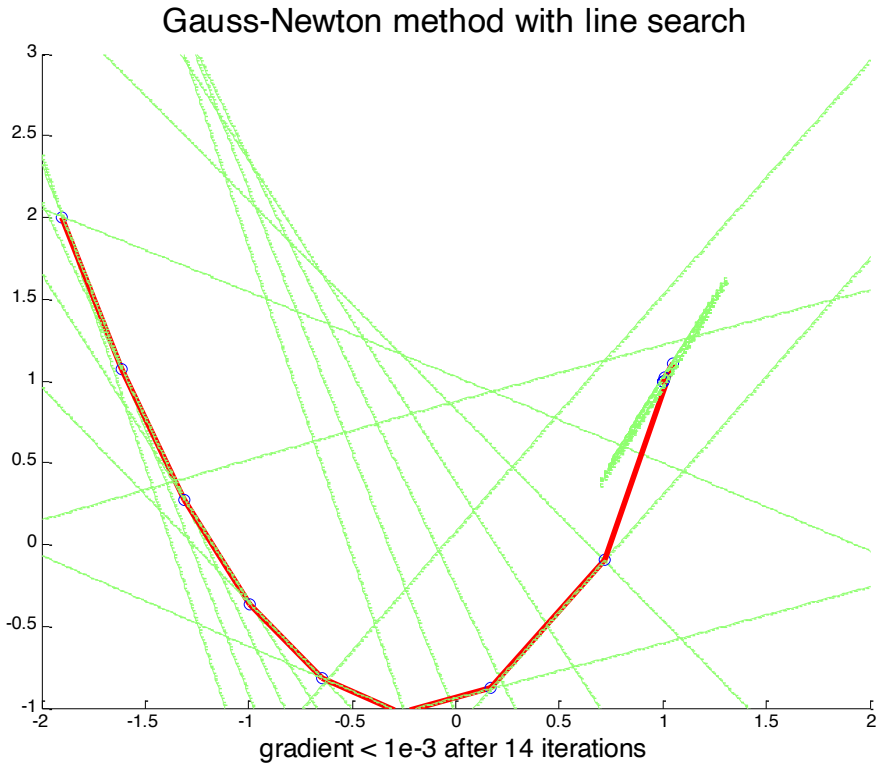
$$\mathrm{J}^T\mathrm{J}\delta\mathbf{x} = -\mathrm{J}^T\mathbf{r}$$

These are called the normal equations.

Gauss-Newton Rosenbrock

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

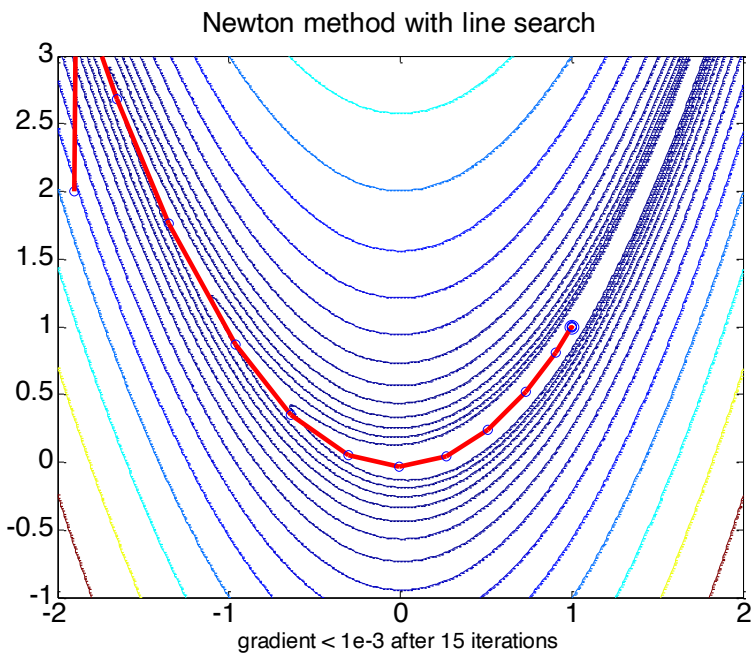




minimization with the Gauss-Newton approximation with line search takes only 14 iterations

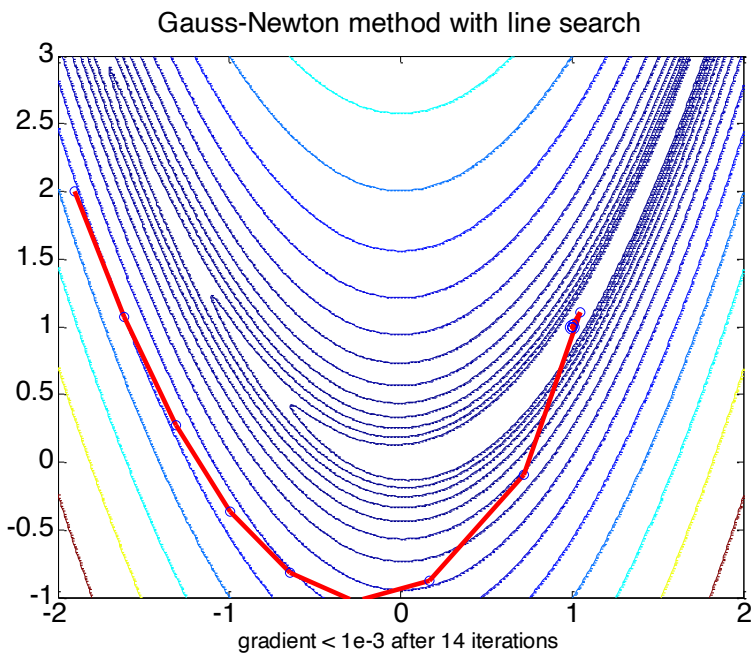
Comparison

Newton



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

Gauss-Newton



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

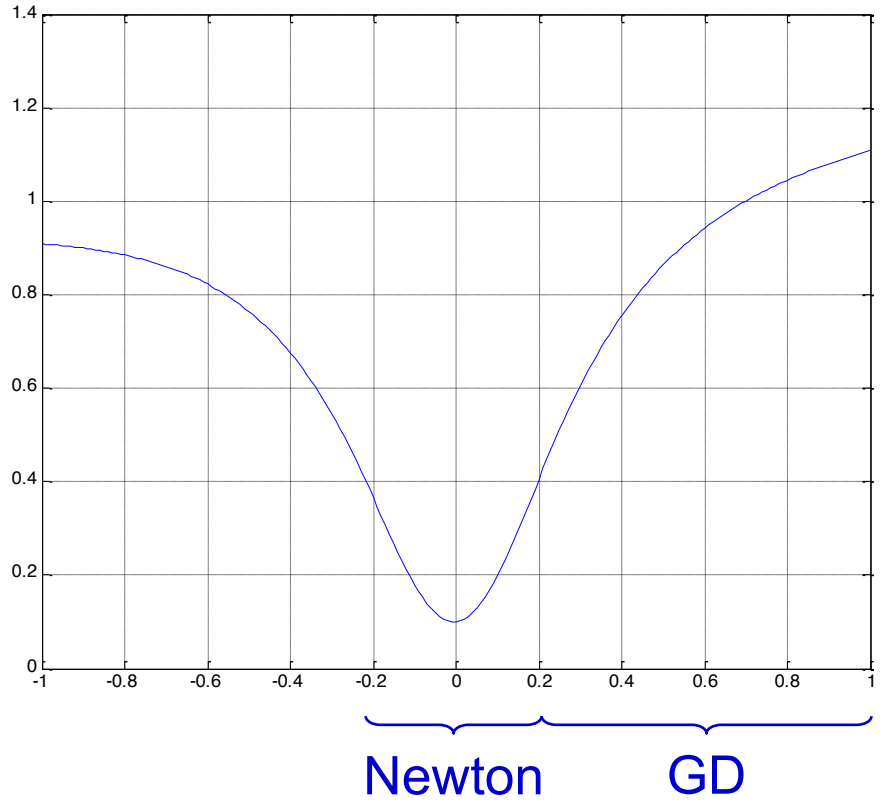
Properties of Methods

Update: $\mathbf{x}_{n+1} = \mathbf{x}_n + \alpha_n \mathbf{p}_n$

- Gradient descent $[\mathbf{p}_n = -\mathbf{g}]$
  - Will zig-zag – each new increment is perpendicular to the previous.
  - Requires 1D search (unless you hack it).
  - Slow to converge.
- Newton's method $[\mathbf{p}_n = -\mathrm{H}^{-1}\mathbf{g}_n]$
  - Requires computation of Hessian.
  - Can converge to maximum or saddle as well as minimum.
  - Can be unstable.
- Gauss-Newton $[\mathrm{p}_n = -\mathrm{H}_{GN}^{-1}\mathbf{g}_n]$
  - Is a downhill method, so will not converge to maximum or saddle.
  - Can be unstable, usually needs line search.

Levenberg-Marquardt [more in C25]

- Away from the minimum, in regions of negative curvature, the Gauss-Newton approximation is not very good.
- In such regions, a simple steepest-descent step is probably the best plan.
- The Levenberg-Marquardt method is a mechanism for varying between steepest-decent and Gauss-Newton steps depending on how good the H_{GN} approximation is locally.



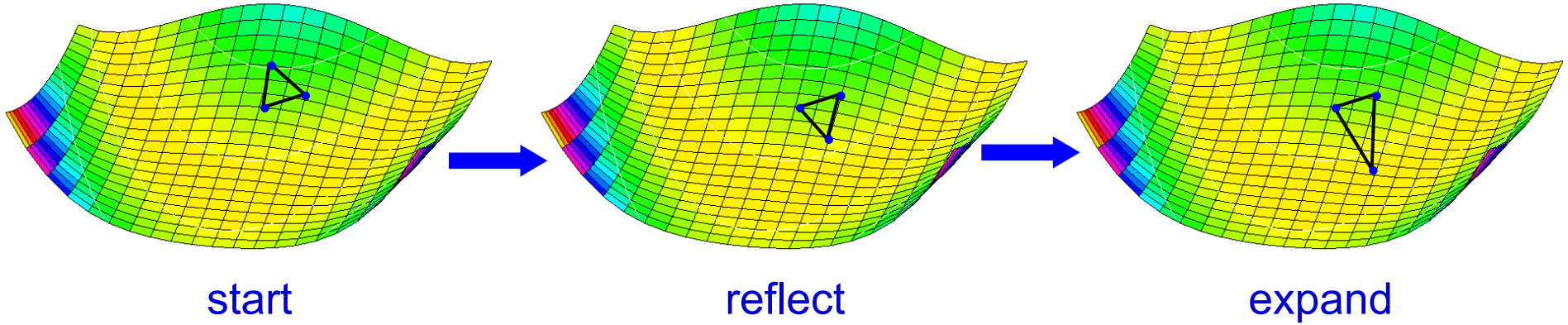
Performance issues for optimization algorithms

1. Number of iterations required
2. Cost per iteration
3. Memory footprint
4. Region of convergence

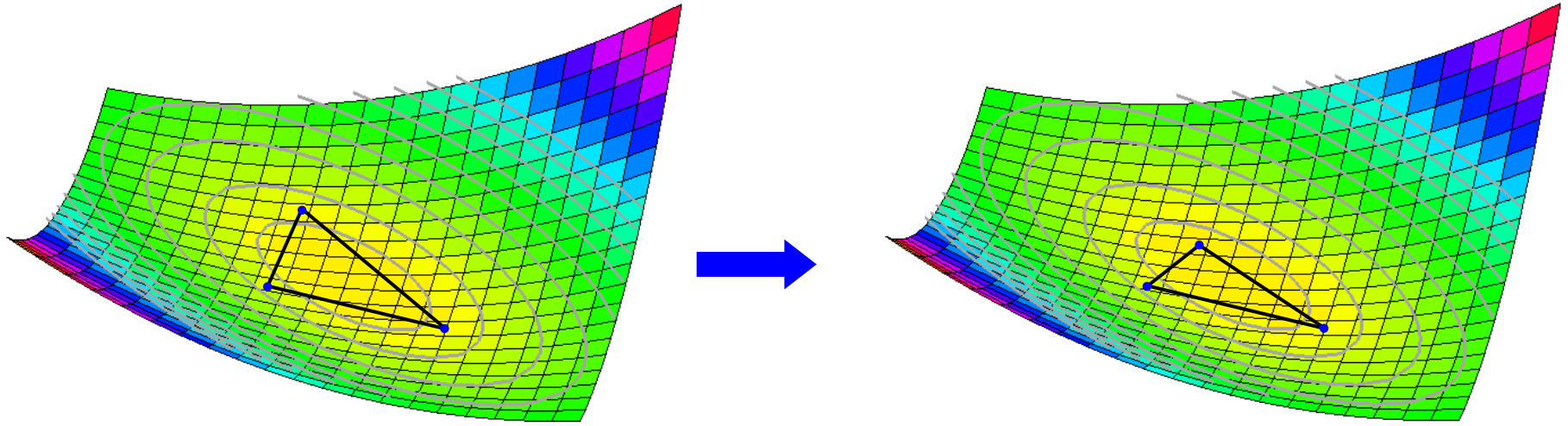
The downhill simplex (amoeba) algorithm

- 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

The downhill simplex (amoeba) algorithm



start reflect expand



contract

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

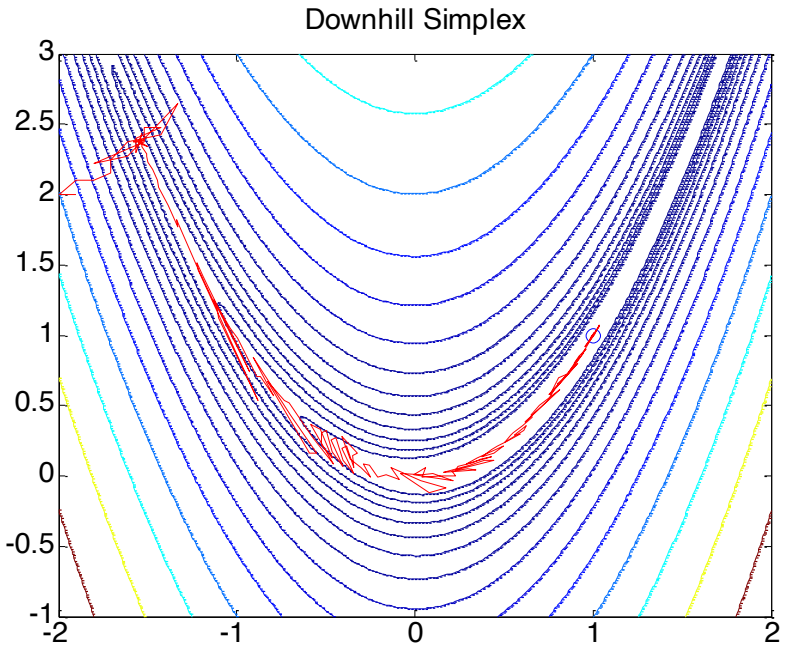
- Calculate $\bar{\mathbf{x}} = (\sum_i \mathbf{x}_i)/N$ as the centroid of all points except $\mathbf{x}_{n+1}$.

- Generate a trial point by reflection $\mathbf{x}_r = \bar{\mathbf{x}} + \alpha(\bar{\mathbf{x}} - \mathbf{x}_{n+1})$, where and $\alpha > 0$.
- If the reflected point $\mathbf{x}_r$ is neither the new best or worst point, i.e. if $f(\mathbf{x}_1) < f(\mathbf{x}_r) < f(\mathbf{x}_n)$ replace the worst point $\mathbf{x}_{n+1}$ by $\mathbf{x}_r$.

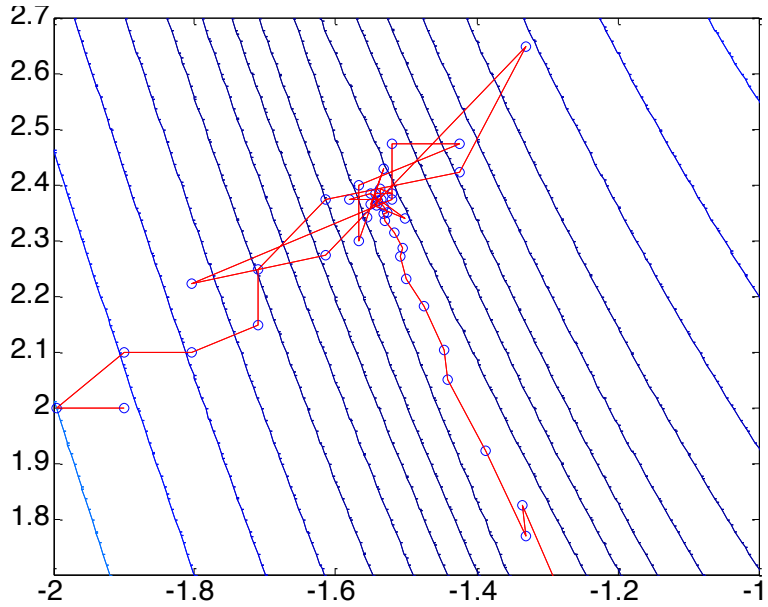
- If the reflected point $\mathbf{x}_r$ is the new best point, i.e. if $f(\mathbf{x}_r) < f(\mathbf{x}_1)$, generate a new point by expansion $\mathbf{x}_e = \mathbf{x}_r + \beta(\mathbf{x}_r - \bar{\mathbf{x}})$, where $\beta > 0$.
- If the expanded point is better than the reflected point $f(\mathbf{x}_e) < f(\mathbf{x}_r)$ then replace $\mathbf{x}_{n+1}$ by $\mathbf{x}_e$, otherwise replace $\mathbf{x}_{n+1}$ by $\mathbf{x}_r$.

- If $f(\mathbf{x}_r) > f(\mathbf{x}_n)$ 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 $\gamma, (0 < \gamma < 1)$ is the contraction coefficient.
- If the contracted point is better than the worst point, so $f(\mathbf{x}_c) < f(\mathbf{x}_{n+1})$, the contraction has succeeded, and replace $\mathbf{x}_{n+1}$ by $\mathbf{x}_c$, otherwise contract again (or shrink all points).

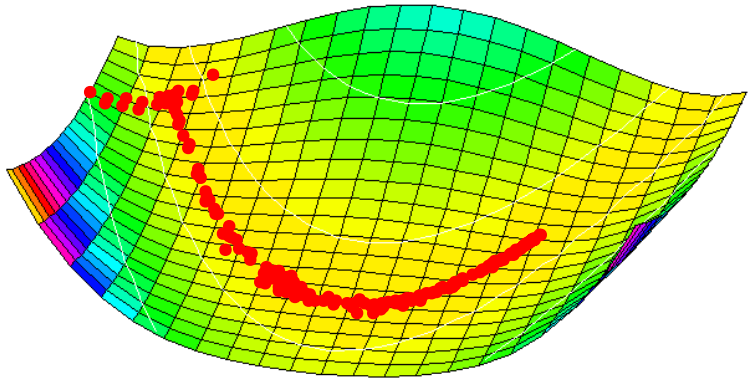
Downhill Simplex Example 1



Path of best vertex

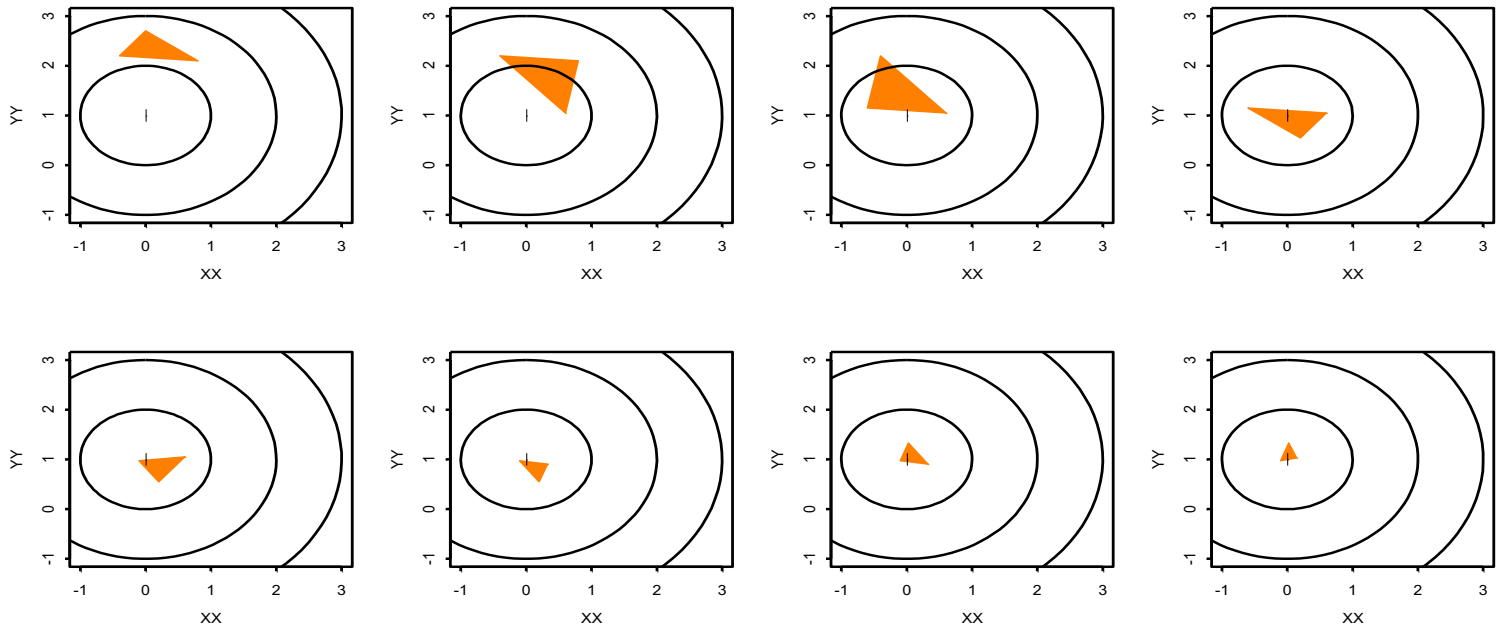


Detail



Matlab fminsearch
with 200 iterations

Downhill Simplex Example 2: Contraction About a Minimum



reflections

contractions

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 optimization.