PHY604 Lecture 11

September 30, 2025

Today's lecture: (non)Linear Algebra

- Eigensystems
- Linear algebra libraries
- Nonlinear algebra: Roots and extrema of multivariable functions

Eigenvalues and eigenvectors

- Very common matrix problem in physics
- Mostly concerned with real symmetric matrices, or Hermitian matrices
- For a symmetric matrix **A**, an eigenvector $\mathbf{v}_i$ satisfies:

$$\mathbf{A}\mathbf{v}_i = \lambda_i \mathbf{v}_i$$

  - λ_i are the eigenvalues
- Eigenvectors are orthogonal, and we will assume they are normalized:

$$\mathbf{v}_i \cdot \mathbf{v}_j = \delta_{ij}$$

- Combining eigenvectors into matrix **V**, and eigenvalues into diagonal matrix **D**:

$$\mathbf{AV} = \mathbf{VD}$$

QR algorithm for calculating eigenvalues/eigenvectors

- We will focus on real, symmetric, square **A**
- Makes use of QR decomposition to obtain **V** and **D**
  - Same idea as LU decomposition
  - Write **A** as a product of orthogonal matrix **Q**, and upper-triangular matrix **R**
  - Any square matrix can be written that way

- 1. Break **A** down into QR decomposition: $\mathbf{A} = \mathbf{Q}_1\mathbf{R}_1$
- 2. Multiply on the left by $\mathbf{Q}_1^\mathrm{T}$:

$$\mathbf{Q}_1^\mathrm{T}\mathbf{A} = \mathbf{Q}_1^\mathrm{T}\mathbf{Q}_1\mathbf{R}_1 = \mathbf{R}_1$$

  - Note that since **Q** is orthogonal, $\mathbf{Q}^\mathrm{T}=\mathbf{Q}^{-1}$

QR decomposition

- 3. Now we define a new matrix, product of $\mathbf{Q}_1$ and $\mathbf{R}_1$ in reverse order:

$$\mathbf{A}_1 = \mathbf{R}_1\mathbf{Q}_1$$

  - Combine with step 2 to get:

$$\mathbf{A}_1 = \mathbf{Q}_1^{\mathrm{T}}\mathbf{A}\mathbf{Q}_1$$

- 4. Repeat the process, find QR decomposition of $\mathbf{A}_1$:

$$\mathbf{A}_2 = \mathbf{R}_2\mathbf{Q}_2 = \mathbf{Q}_2^{\mathrm{T}}\mathbf{A}_1\mathbf{Q}_2 = \mathbf{Q}_2^{\mathrm{T}}\mathbf{Q}_1^{\mathrm{T}}\mathbf{A}\mathbf{Q}_1\mathbf{Q}_2$$

  - And so on:

$$\begin{aligned}
\mathbf{A}_1 &= \mathbf{Q}_1^{\mathrm{T}}\mathbf{A}\mathbf{Q}_1 \\
\mathbf{A}_2 &= \mathbf{Q}_2^{\mathrm{T}}\mathbf{Q}_1^{\mathrm{T}}\mathbf{A}\mathbf{Q}_1\mathbf{Q}_2 \\
\mathbf{A}_3 &= \mathbf{Q}_3^{\mathrm{T}}\mathbf{Q}_2^{\mathrm{T}}\mathbf{Q}_1^{\mathrm{T}}\mathbf{A}\mathbf{Q}_1\mathbf{Q}_2\mathbf{Q}_3 \\
&\vdots \\
\mathbf{A}_k &= (\mathbf{Q}_k^{\mathrm{T}}\dots\mathbf{Q}_1^{\mathrm{T}})\mathbf{A}(\mathbf{Q}_1\dots\mathbf{Q}_k)
\end{aligned}$$

Eigenvalues and eigenvectors from QR decomposition

- If you continue this process long enough, the matrix $\mathbf{A}_k$ will eventually become diagonal:

$$\mathbf{A}_k \simeq \mathbf{D}$$

- Continue until the off-diagonal elements are below some accuracy
- Eigenvector matrix is given by:

$$\mathbf{V} = \mathbf{Q}_1\mathbf{Q}_2\mathbf{Q}_3\ldots\mathbf{Q}_k = \prod_{i=1}^{k}\mathbf{Q}_i$$

- **V** Orthogonal since the product of orthogonal matrices is orthogonal. Then:

$$\mathbf{D} = \mathbf{A}_k = \mathbf{V}^{\mathrm{T}}\mathbf{A}\mathbf{V}$$

- So:

$$\mathbf{A}\mathbf{V} = \mathbf{V}\mathbf{D}$$

How do we do the QR decomposition?

- Think of the matrix as a set of *N* columns:

$$\mathbf{A} = \begin{pmatrix} | & | & | & \cdots \\ \mathbf{a}_0 & \mathbf{a}_1 & \mathbf{a}_2 & \cdots \\ | & | & | & \cdots \end{pmatrix}$$

- Now define two new sets of vectors:

$$\mathbf{u}_0 = \mathbf{a}_0, \qquad \mathbf{q}_0 = \frac{\mathbf{u}_0}{|\mathbf{u}_0|}$$

$$\mathbf{u}_1 = \mathbf{a}_1 - (\mathbf{q}_0 \cdot \mathbf{a}_1)\mathbf{q}_0, \qquad \mathbf{q}_1 = \frac{\mathbf{u}_1}{|\mathbf{u}_1|}$$

$$\mathbf{u}_2 = \mathbf{a}_2 - (\mathbf{q}_0 \cdot \mathbf{a}_2)\mathbf{q}_0 - (\mathbf{q}_1 \cdot \mathbf{a}_2)\mathbf{q}_1, \qquad \mathbf{q}_2 = \frac{\mathbf{u}_2}{|\mathbf{u}_2|}$$

$$\vdots \qquad \vdots$$

(Gram-Schmidt orthogonalization!)

How do we do the QR decomposition?

- General formula for $\mathbf{u}_i$ and $\mathbf{q}_i$:

$$\mathbf{u}_i = \mathbf{a}_i - \sum_{j=0}^{i-1} (\mathbf{q}_j \cdot \mathbf{a}_i)\mathbf{q}_j, \qquad \mathbf{q}_i = \frac{\mathbf{u}_i}{|\mathbf{u}_i|}$$

- We can show that the **q** vectors are orthonormal:

$$\mathbf{q}_i \cdot \mathbf{q}_j = \delta_{ij}$$

- Now we rearrange the definitions of the vectors:

$$\mathbf{a}_0 = |\mathbf{u}_0|\mathbf{q}_0,$$
$$\mathbf{a}_1 = |\mathbf{u}_1|\mathbf{q}_1 + (\mathbf{q}_0 \cdot \mathbf{a}_1)\mathbf{q}_0$$
$$\mathbf{a}_2 = |\mathbf{u}_2|\mathbf{q}_2 + (\mathbf{q}_0 \cdot \mathbf{a}_2)\mathbf{q}_0 + (\mathbf{q}_1 \cdot \mathbf{a}_2)\mathbf{q}_1$$

How do we do the QR decomposition?

- Finally write all the equations as a single matrix equation:

$$\mathbf{A} = \begin{pmatrix} | & | & | & \dots \\ \mathbf{a}_0 & \mathbf{a}_1 & \mathbf{a}_2 & \dots \\ | & | & | & \dots \end{pmatrix} = \begin{pmatrix} | & | & | & \dots \\ \mathbf{q}_0 & \mathbf{q}_1 & \mathbf{q}_2 & \dots \\ | & | & | & \dots \end{pmatrix} \begin{pmatrix} |\mathbf{u}_0| & \mathbf{q}_0 \cdot \mathbf{a}_1 & \mathbf{q}_0 \cdot \mathbf{a}_2 & \dots \\ 0 & |\mathbf{u}_1| & \mathbf{q}_1 \cdot \mathbf{a}_2 & \dots \\ 0 & 0 & |\mathbf{u}_2| & \dots \end{pmatrix}$$

- Our QR decomposition is thus

$$\mathbf{Q} = \begin{pmatrix} | & | & | & \dots \\ \mathbf{q}_0 & \mathbf{q}_1 & \mathbf{q}_2 & \dots \\ | & | & | & \dots \end{pmatrix}, \qquad \mathbf{R} = \begin{pmatrix} |\mathbf{u}_0| & \mathbf{q}_0 \cdot \mathbf{a}_1 & \mathbf{q}_0 \cdot \mathbf{a}_2 & \dots \\ 0 & |\mathbf{u}_1| & \mathbf{q}_1 \cdot \mathbf{a}_2 & \dots \\ 0 & 0 & |\mathbf{u}_2| & \dots \end{pmatrix}$$

- **Q** is orthogonal since the columns are orthonormal
- **R** is upper triangular

QR decomposition algorithm:

- For a give *N* x *N* starting matrix **A**:

- 1. Create an *N* x *N* array to hold **V**; initialize as identity
- 2. Calculate QR decomposition **A** = **QR**
- 3. Update **A** with new value **A** = **RQ**
- 4. Multiply **V** on the RHS with **Q**
- 5. Check off-diagonal elements of **A**. If they are less than some tolerance, we are done. Otherwise go back to 2.

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Libraries for linear algebra: BLAS (basic linear algebra subroutines)

- These are the standard building blocks (API) of linear algebra on a computer (Fortran and C)
- Most linear algebra packages formulate their operations in terms of BLAS operations
- Three levels of functionality:
  - Level 1: vector operations ($\alpha \mathbf{x} + \mathbf{y}$)
  - Level 2: matrix-vector operations ($\alpha \mathbf{A}\,\mathbf{x} + \beta\,\mathbf{y}$)
  - Level 3: matrix-matrix operations ($\alpha \mathbf{A}\,\mathbf{B} + \beta\,\mathbf{C}$)
- Available on pretty much every platform (http://www.netlib.org/blas/)
  - See (https://en.wikipedia.org/wiki/Basic_Linear_Algebra_Subprograms)
  - Some compilers provide specially optimized BLAS libraries (-lblas) that take great advantage of the underlying processor instructions
  - ATLAS: automatically tuned linear algebra software

Libraries for linear algebra: LAPACK

- The standard for linear algebra
- Built upon BLAS
- Routines named in the form xyyzzz
  - x refers to the data type (s/d are single/double precision floating, c/z are single/double complex)
  - yy refers to the matrix type
  - zzz refers to the algorithm (e.g. sgebrd = single precision bi-diagonal reduction of a general matrix)

- Routines: https://github.com/Reference-LAPACK/lapack/tree/master

Libraries for linear algebra: Python

- Basic methods in numpy.linalg (based on BLAS and LAPACK)
  - https://numpy.org/doc/stable/reference/routines.linalg.html
  - Has a matrix type built from the array class
  - * operator works element by element for arrays but does matrix product for matrices
  - As of python 3.5, @ operator will do matrix multiplication for NumPy arrays
  - Vectors are automatically converted into 1×N or N×1 matrices
  - Matrix objects cannot be > rank 2
  - Matrix has .H (or .T), .I, and .A attributes (transpose, inverse, as array)

- More general stuff in SciPy (scipy.linalg)
  - http://docs.scipy.org/doc/scipy/reference/linalg.html

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Multivariate Newton's method

- We can generalize Newton's method for equations with several variables
  - Can be used when we no longer have a linear system
  - Cast the problem as one of root finding
- Consider the vector function: $\mathbf{f}(\mathbf{x}) = \begin{bmatrix} f_1(\mathbf{x}) & f_1(\mathbf{x}) & \ldots & f_N(\mathbf{x}) \end{bmatrix}$
- Where the unknowns are: $\mathbf{x} = \begin{bmatrix} x_1 & x_1 & \ldots & x_N \end{bmatrix}$
- Revised guess from initial guess $\mathbf{x}^{(0)}$: $\mathbf{x}_1 = \mathbf{x}_0 - \mathbf{f}(\mathbf{x}_0)\mathbf{J}^{-1}(\mathbf{x}_0)$
  - $\mathbf{J}^{-1}$ is the inverse of the Jacobian matrix:

$$J_{ij}(\mathbf{x}) = \frac{\partial f_i(\mathbf{x})}{\partial x_i}$$

- To avoid taking the inverse at each step, solve with Gaussian substitution:

$$\mathbf{J}\delta\mathbf{x}^k = -\mathbf{f}(\mathbf{x}^k)$$

Example: Lorenz model (Garcia Sec. 4.3)

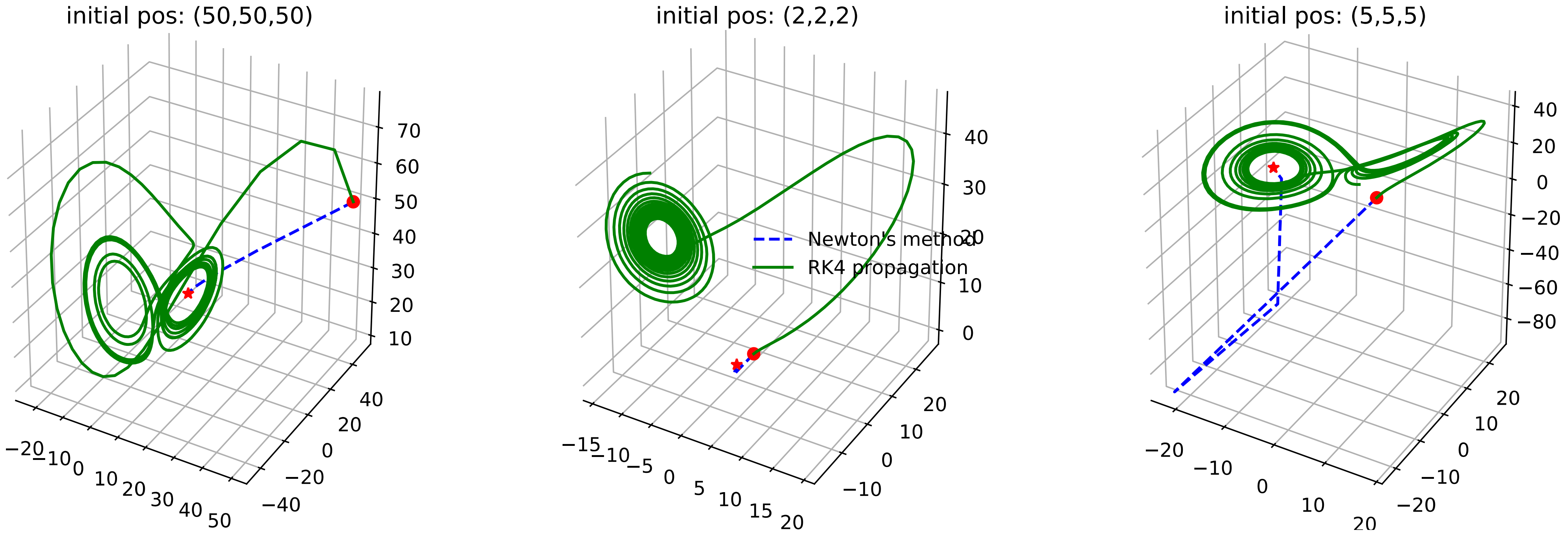
- Lorenz system:

$$\frac{dx}{dt} = \sigma(y - x)$$
$$\frac{dy}{dt} = rx - y - xz$$
$$\frac{dz}{dt} = xy - bz$$

- σ, *r*, and *b* are positive constants
- If we want steady-state, we can propagate with, e.g., 4^{th} order RK
- Steady-state directly given by roots of Lorenz system:

$$\mathbf{f}(x, y, z) = \begin{pmatrix} \sigma(y - x) \\ rx - y - xz \\ xy - bz \end{pmatrix} = 0 \qquad \mathbf{J} = \begin{pmatrix} -\sigma & \sigma & 0 \\ r - z & -1 & -x \\ y & x & -b \end{pmatrix}$$

Lorenz model steady-state: Newton versus 4th order RK



Steepest descent: Extrema of multivariable functions

- Used for finding roots, minima, or maxima of functions of several variables
- Based on the idea of moving downhill with each iteration, i.e., opposite to the gradient
  - If current position is $\mathbf{x}_n$, next step is:

$$x_{n+1} = x_n - \alpha_n \nabla f(x_n)$$

- Determine the step size α such that we reach the line minimum in direction of the gradient:

$$\frac{d}{d\alpha_n} f[x_{n+1}(\alpha_n)] = -\nabla f(x_{n+1}) \cdot \nabla f(x_n) = 0$$

- Find root of function of α :

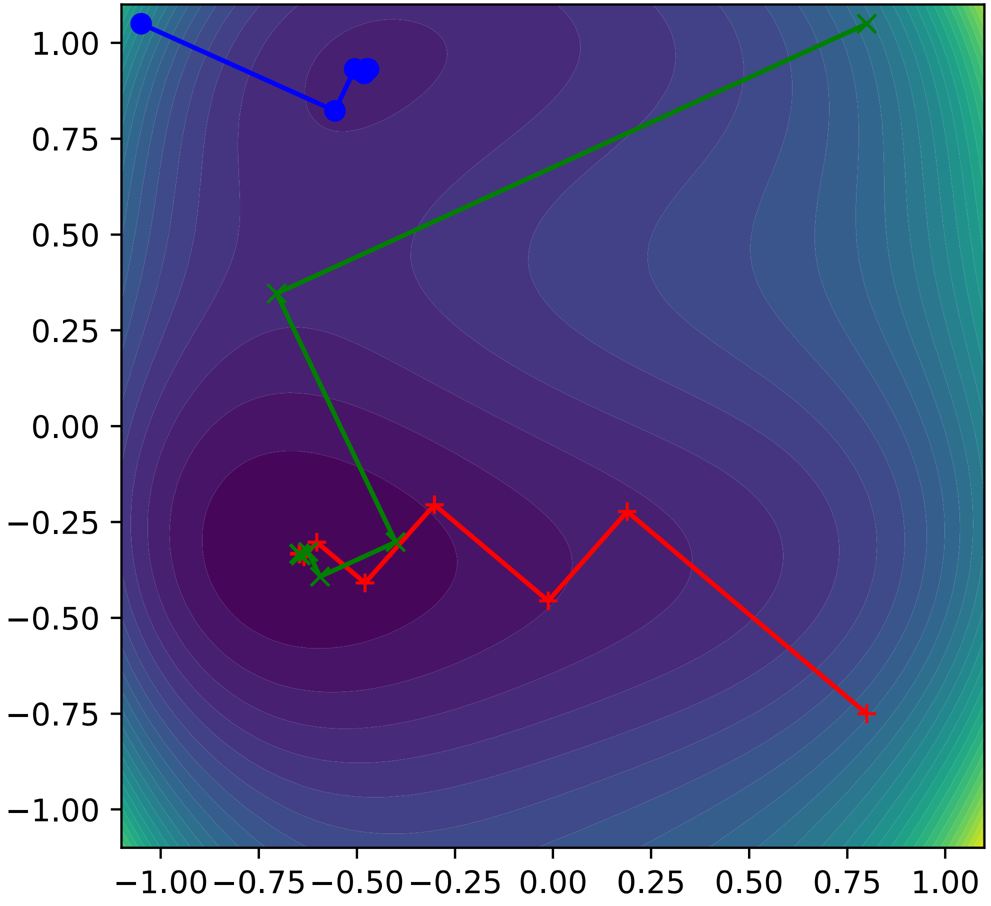
$$g(\alpha) = \nabla f[x_{n+1}(\alpha)] \cdot \nabla f(x_n) = 0$$

Steepest descent example

(From Stickler and Schachinger: Basic Concepts in Computational Physics)

- Consider the function:

$$f(x, y) = \cos(2x) + \sin(4y) + \exp(1.5x^2 + 0.7y^2) + 2x$$



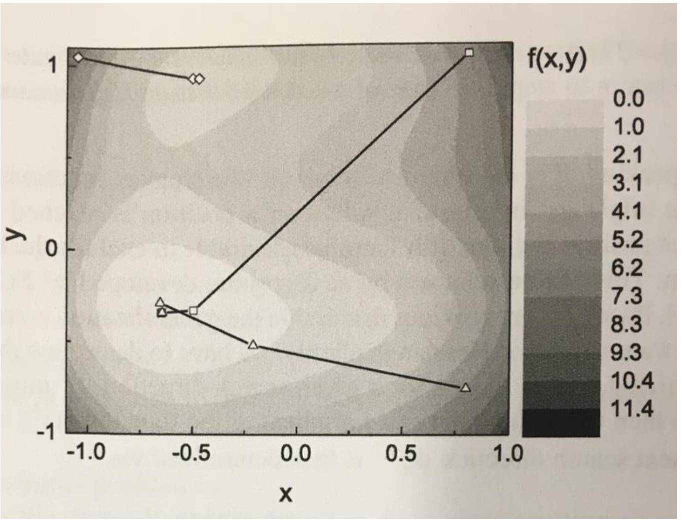
Comments on steepest descent

- Rather slow due to orthogonality of subsequent search directions
- Can only find local minimum closest to starting point
  - Not global minimum
- Convergence rate is highly affected by choice of initial position
- Very simple method, works in space of arbitrary dimensions

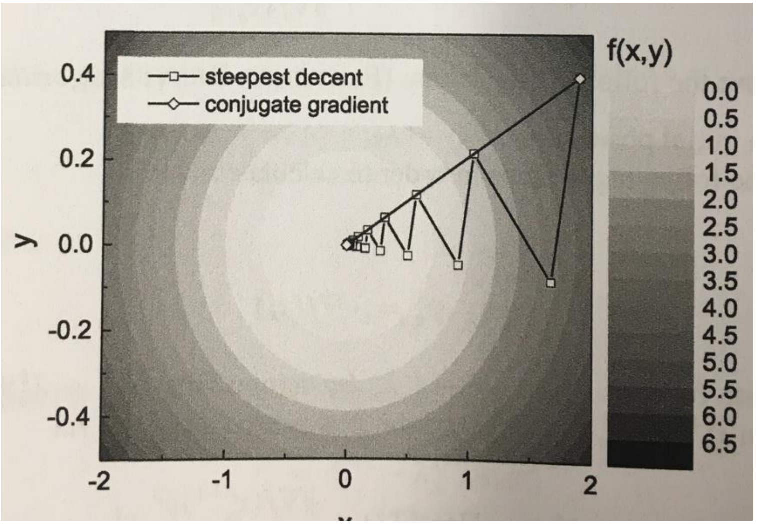
Conjugate gradients method

- Based on the definition of *N* orthogonal search directions in *N* dimensional space
- Consider function in "quadratic" form: $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} - \mathbf{b}^{\mathrm{T}}\mathbf{x} + c$
- For functions in this form, CG method will converge in at most *N* steps
  - More steps for general functions, still more efficient than steepest descent
- Formulation is a bit complex, see readings

Previous slide example



$f(x,y) = x^2 + 10y^2$



Stickler and Schachinger

After class tasks

- Homework 2 due tomorrow Oct. 1 by the end of the day

- **Class on Thursday Oct. 2 will start at late at 2:30pm!**

- Readings:
  - Newman Ch. 6
  - Garcia Ch. 4
  - Pang Ch. 5

  - "An Introduction to the Conjugate Gradient Method Without the Agonizing Pain," Jonathan Richard Shewchuk