Nonlinear Least Squares

1. Gauss-Newton Method
   - nonlinear overdetermined systems
   - near intersection points of three circles
   - a computation with Julia
2. Singular Value Decomposition
   - yet another matrix factorization ...
   - computing the condition number of a matrix
3. Levenberg-Marquardt Method
   - adding a regularization term
   - description of the method

MCS 471 Lecture 21
Numerical Analysis
Jan Verschelde, 10 October 2022

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nonlinear overdetermined systems

Let $\mathbf{f} = (f_1, f_2, \ldots, f_m)$ define the overdetermined system $\mathbf{f}(\mathbf{x}) = \mathbf{0}$, with

1. m equations $f_i(\mathbf{x}) = 0$, $i = 1, 2, \ldots, m$,
2. in n variables $\mathbf{x} = (x_1, x_2, \ldots, x_n)$.

where $m > n$.

Solving $\mathbf{f}(\mathbf{x}) = \mathbf{0}$ in the least squares sense
means finding a solution $\mathbf{z} = (z_1, z_2, \ldots, z_n)$ such that

$$\|\mathbf{f}(\mathbf{z})\|_2^2 = f_1(\mathbf{z})^2 + f_2(\mathbf{z})^2 + \cdots + f_m(\mathbf{z})^2$$

is minimal. $\|\mathbf{f}(\mathbf{z})\|_2$ is the norm of the residual, or backward error.

There may be many solutions of $\mathbf{f}(\mathbf{x}) = \mathbf{0}$.

the Jacobian matrix

We need the matrix of all first order partial derivatives

$$J_{\mathbf{f}} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \frac{\partial f_m}{\partial x_2} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}.$$

$J_{\mathbf{f}}$ is the Jacobian matrix of the system $\mathbf{f}(\mathbf{x}) = \mathbf{0}$.

For a system $\mathbf{f}(\mathbf{x}) = \mathbf{0}$ of m equations in n variables, $J_{\mathbf{f}}$ is an m-by-n matrix.

one Gauss-Newton step

Given are $\mathbf{f}(\mathbf{x}) = \mathbf{0}$ and $\mathbf{x}_0 \in \mathbb{R}^n$.
The $\mathbf{x}_0$ contains approximations for the coordinates of a solution.

1. Evaluate $\mathbf{f}$ at $\mathbf{x}_0$, $\mathbf{b} := -\mathbf{f}(\mathbf{x}_0)$.
2. Evaluate $J_{\mathbf{f}}$ at $\mathbf{x}_0$, $A := J_{\mathbf{f}}(\mathbf{x}_0)$.
3. Solve $A\Delta\mathbf{x} = \mathbf{b}$.
4. Update $\mathbf{x}_0$: $\mathbf{x}_1 := \mathbf{x}_0 + \Delta\mathbf{x}$.

Consider the linear system $A\Delta\mathbf{x} = \mathbf{b}$:

- As $\mathbf{f}$ defines m equations, $\mathbf{b} \in \mathbb{R}^m$.
- Since $J_{\mathbf{f}}$ is an m-by-n matrix, with $m > n$, the matrix A is also m-by-n.

We solve $A\Delta\mathbf{x} = \mathbf{b}$ in the least squares sense, preferably with a QR factorization.

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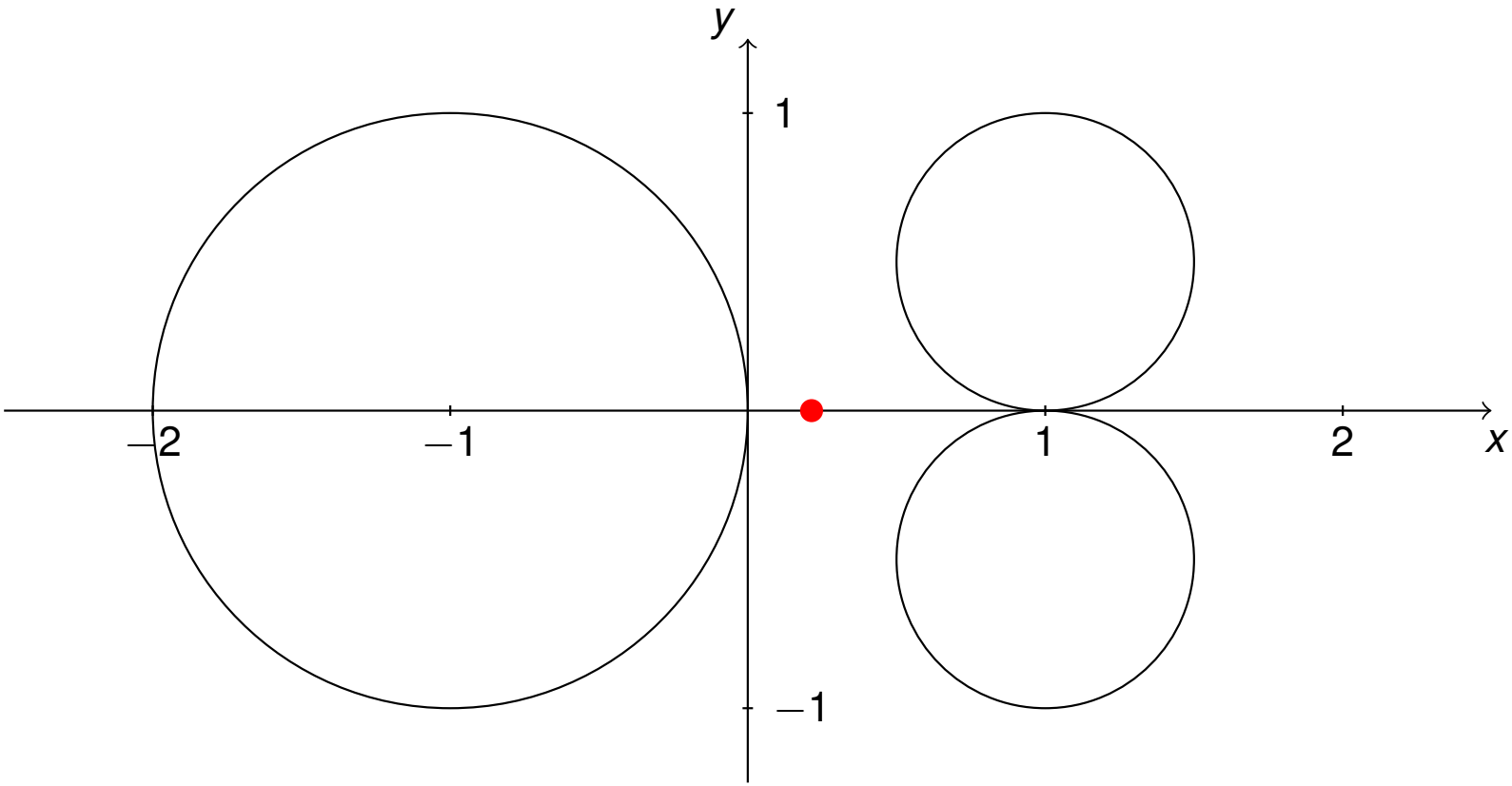
near intersection points of three circles



$$\text{minimize} \sum_{k=1}^{3} \left(\sqrt{(x - x_k)^2 + (y - y_k)^2} - r_k \right)^2$$

a system of nonlinear equations

$$\text{minimize} \sum_{k=1}^{3} \left(\sqrt{(x-x_k)^2 + (y-y_k)^2} - r_k \right)^2$$

for $(x_1, y_1) = (-1, 0)$, $r_1 = 1$,
$(x_2, y_2) = (1, 0.5)$, $r_2 = 0.5$, and
$(x_3, y_3) = (1, -0.5)$, $r_3 = 0.5$.

We apply the method of Gauss-Newton to

$$\begin{cases} \sqrt{(x+1)^2 + y^2} - 1 &= 0 \\ \sqrt{(x-1)^2 + (y-0.5)^2} - 0.5 &= 0 \\ \sqrt{(x-1)^2 + (y+0.5)^2} - 0.5 &= 0. \end{cases}$$

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a computation with Julia

Recall the script `multinewton.jl` from Lecture L-13.

In the function `main()`, we define the equations as

```
one = "sqrt((x+1)*(x+1) + y*y) - 1"
two = "sqrt((x-1)*(x-1) + (y-0.5)*(y-0.5)) - 0.5"
three = "sqrt((x-1)*(x-1) + (y+0.5)*(y+0.5)) - 0.5"
```

The other adjustments consists in adding a third `h`
next to the `f` and `g` equations.

the same function `NewtonStep`

```
"""
Does one step of the Gauss-Newton method,
on the vector function fun and Jacobian jac,
starting at x0, y0.  Returns the new values
for x and y, the norm of the update, and
the norm of the residual at x0, y0.
"""
function NewtonStep(fun, jac,
                    x0::Float64, y0::Float64)
    valfun = -SymPyFun(fun, x0, y0)
    nfx = norm(valfun)
    valmat = SymPyMatrixEvaluate(jac, x0, y0)
    update = valmat\valfun
    ndx = norm(update)
    x1 = x0 + update[1]
    y1 = y0 + update[2]
    return [x1, y1, ndx, nfx]
end
```

running `NewtonStep`

Starting at $(0, 0)$, we print after each step

1. x, the value of the first coordinate of the solution
2. y, the value of the second coordinate of the solution
3. $\|(\Delta x, \Delta y)\|_2$, the norm of the update, estimates the forward error
4. $\|\mathbf{f}(x, y)\|_2$, the norm of the residual, estimates the backward error

```
step                x                               y                  |update|    |f(x,y)|
  0 :  0.0000000000000000e+00   0.0000000000000000e+00
  1 :  4.2522031115387854e-01   8.7770836714417518e-17  4.25e-01    8.74e-01
  2 :  4.1112530855930013e-01  -9.1648644610152970e-17  1.41e-02    5.64e-01
  3 :  4.1313149307582292e-01   1.5093412638940774e-16  2.01e-03    5.64e-01
  4 :  4.1285833541953565e-01  -3.0643041052992871e-17  2.73e-04    5.64e-01
  5 :  4.1289576405778744e-01   9.0441053455228248e-17  3.74e-05    5.64e-01
  6 :  4.1289063992215830e-01  -9.1178377175993533e-17  5.12e-06    5.64e-01
  7 :  4.1289134152035289e-01   2.1152220516108437e-16  7.02e-07    5.64e-01
  8 :  4.1289124545886885e-01  -1.5171824204619955e-16  9.61e-08    5.64e-01
  9 :  4.1289125861145282e-01   1.5098215933337173e-16  1.32e-08    5.64e-01
 10 :  4.1289125681062272e-01  -3.0638079136074756e-17  1.80e-09    5.64e-01
```

Why so slow?

convergence of the Gauss-Newton method

With the backslash operator, Gauss-Newton is the same as Newton.

- The initial point must be close enough to the solution.
- If the solution makes all equations zero,
  then we may expect quadratic convergence.

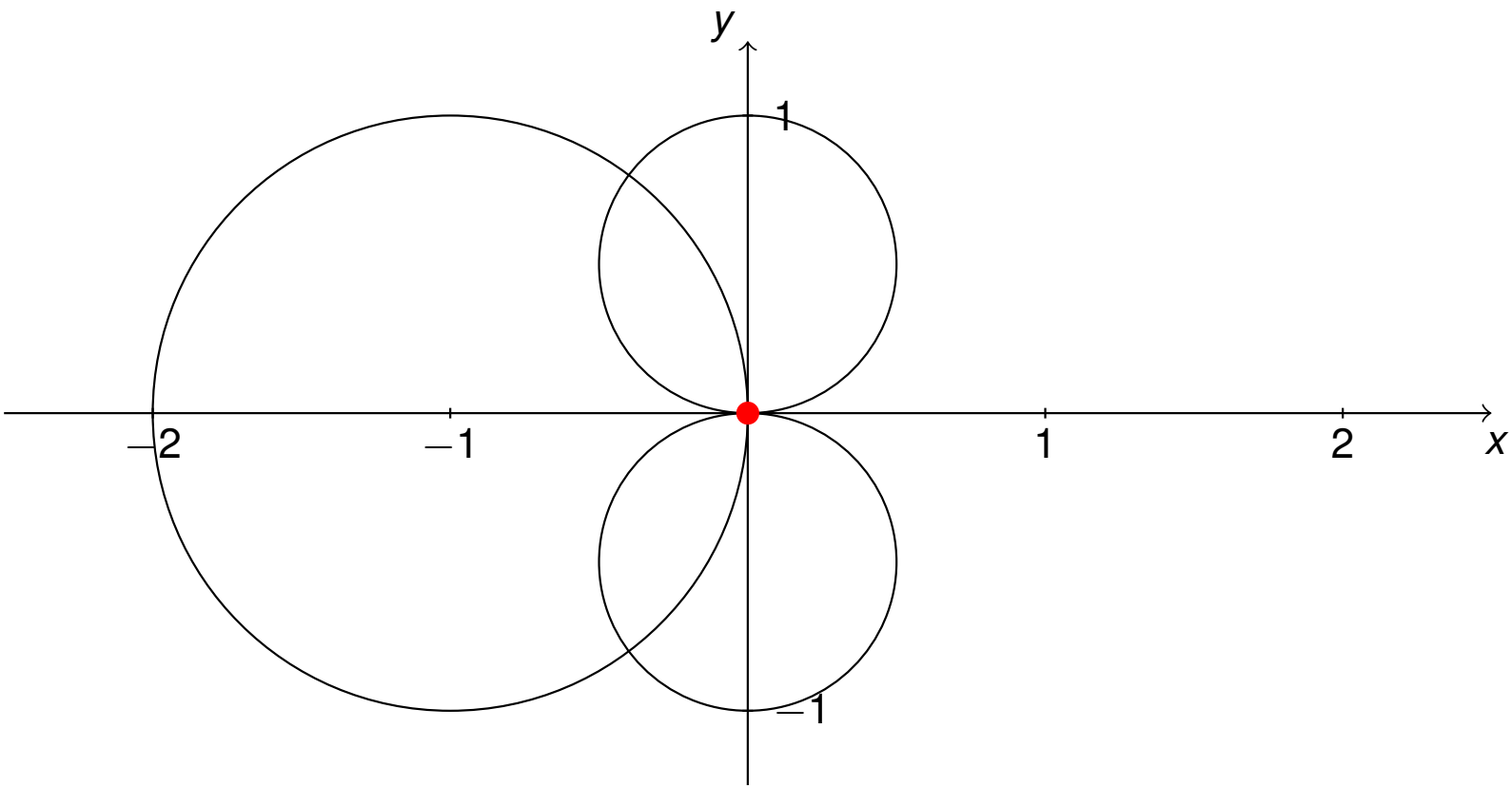
Gauss-Newton differs from Newton

- if there is *no* solution that makes all equations zero, or
- if there is only a least squares solution.

If the overconstrained problem is then *well posed*,
then we may expect local, linear convergence.

the intersection point of three circles

Exercise 1: Consider the modification of the three circle problem:



The centers of the two smaller circles are at $(0, \pm 0.5)$.
Run the method of Gauss-Newton, starting at $(0.5, 0.0)$.
Is the convergence quadratic?

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the Singular Value Decomposition

Let A by an n-by-k matrix, $k \leq n$.

The Singular Value Decomposition (SVD) of A is defined by

1. U, an n-by-n orthogonal matrix, $U^T U = I$,
2. S, a diagonal n-by-k matrix with the singular values, and
3. V, is an k-by-k orthogonal matrix, $V^T V = I$,

such that $A = USV^T$ or equivalently: $U^T AV = S$.

Two important properties of the SVD.

1. The SVD provides a *diagonalization of A*, it generalizes QR.
2. The singular values are sorted in descending order.
   Given a tolerance ϵ, *the numerical rank of A*
   equals the number of singular values larger than ϵ.

the `svd` in a Julia session

```
julia> using LinearAlgebra

julia> A = rand(3, 2)
3×2 Array{Float64,2}:
 0.887977  0.173145
 0.768222  0.971541
 0.346458  0.481141

julia> U, S, V = svd(A)
SVD{Float64,Float64,Array{Float64,2}}
U factor:
3×2 Array{Float64,2}:
 -0.502462   0.863655
 -0.781218  -0.433491
 -0.370447  -0.257265
singular values:
2-element Array{Float64,1}:
 1.558484008477351
 0.5245922051038863
Vt factor:
2×2 Array{Float64,2}:
 -0.753724  -0.657191
  0.657191  -0.753724
```

verification of the properties

The session with Julia continues:

```
julia> A
3×2 Array{Float64,2}:
 0.887977  0.173145
 0.768222  0.971541
 0.346458  0.481141

julia> U*diagm(S)*transpose(V)
3×2 Array{Float64,2}:
 0.887977  0.173145
 0.768222  0.971541
 0.346458  0.481141

julia> transpose(U)*A*V
2×2 Array{Float64,2}:
 1.55848       4.44089e-16
 3.88578e-16   0.524592
```

Indeed, $USV^T = A$ and $U^T AV = S$.

last output of the three circle problem

After 10 iterations with Gauss-Newton on the problem of intersecting three circles, we end with $\|\Delta x\| = 1.80 \cdot 10^{-9}$.

Evaluating the solution then at the Jacobian matrix and computing the singular values shows:

```
The Jacobian matrix :
3x2 Array{Float64,2}:
   1.000e+00  -2.168e-17
  -7.613e-01  -6.484e-01
  -7.613e-01   6.484e-01
The singular values of the Jacobian matrix :
2-element Array{Float64,1}:
 1.469e+00
 9.169e-01
```

We see that the columns of the Jacobian matrix are linearly independent, which shows in the two nonzero singular values. So the problem of intersecting three circles is well posed.

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computing the condition number of a matrix

For square matrices A, we derived $\kappa(A) = \|A^{-1}\|\|A\|$ as the condition number of the matrix A.

But what if A is not square and A^{-1} does not exist?

Let A by an n-by-k matrix, $k \leq n$, and $A = USV^T$.

The k singular values of A are $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_k$.

Then the condition number $\kappa(A)$ of A is

$$\kappa(A) = \frac{\sigma_1}{\sigma_k},$$

provided $\sigma_k \neq 0$.

verification in a Julia session

```
julia> A = rand(3,3)
3×3 Array{Float64,2}:
 0.296377  0.311904   0.777915
 0.648831  0.316846   0.207123
 0.485538  0.0975773  0.837667

julia> cond(A)
7.296520716757458

julia> U, S, V = svd(A);

julia> S
3-element Array{Float64,1}:
 1.4224222554304933
 0.4901166427005800 3
 0.1949452774339017

julia> S[1]/S[3]
7.296520716757455
```

solving linear systems in the least squares sense

If $A = USV^T$, then $A\mathbf{x} = \mathbf{b}$ turns into $USV^T\mathbf{x} = \mathbf{b}$, or $S\mathbf{y} = U^T\mathbf{b}$, with $\mathbf{y} = V^T\mathbf{x}$ or $\mathbf{x} = V\mathbf{y}$.

The above formulas can be used to solve $A\mathbf{x} = \mathbf{b}$.

Exercise 2:

Consider the system $A\mathbf{x} = \mathbf{b}$ with $A = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{bmatrix}$, and $\mathbf{b} = \begin{bmatrix} 1 \\ 2 \\ 0 \end{bmatrix}$.

Compute the singular value decomposition of A and use it to solve $A\mathbf{x} = \mathbf{b}$.

Compare your result with the output of $\mathbf{x} = A\backslash\mathbf{b}$.

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adding a regularization term

To remedy the conditioning of the normal equations, we use a regularization parameter λ.

Let $A = J_{\mathbf{f}}(\mathbf{x}_0)$, instead of $A\Delta\mathbf{x} = -\mathbf{f}(\mathbf{x}_0)$, consider

$$\left(A^T A + \lambda \text{diag}(A^T A)\right)\mathbf{v} = -A^T \mathbf{f}(\mathbf{x}_0)$$

followed by $\mathbf{x}_1 := \mathbf{x}_0 + \mathbf{v}$.

Two extreme cases are interesting:

1. $\lambda = 0$: Gauss-Newton,
2. $\lambda = \infty$: method of steepest descent.

the condition of $A^T A + \lambda \text{diag}(A^T A)$

Exercise 3:
Compare the condition number of $A^T A$
with the condition number of $A^T A + \lambda \text{diag}(A^T A)$,
for random square matrices A of prescribed condition number 10^8.

Experiment with values $\lambda = 1, 10^{-2}, 10^{-4}, 10^{-6}$
and report the observed condition numbers of $A^T A + \lambda \text{diag}(A^T A)$.

Based on your experiments, could you describe the relationship between $\kappa(A^T A)$ and $\kappa(A^T A + \lambda \text{diag}(A^T A))$?

the gradient vector

Note that we want to minimize the square of the residual:

$$r(x,y) = f_1(x,y)^2 + f_2(x,y)^2 + f_3(x,y)^2.$$

The critical points are solutions of $\frac{\partial r}{\partial x} = 0$ and $\frac{\partial r}{\partial y} = 0$.

$$\begin{aligned}
\frac{\partial r}{\partial x} &= 2f_1(x,y)\frac{\partial f_1}{\partial x} + 2f_2(x,y)\frac{\partial f_2}{\partial x} + 2f_3(x,y)\frac{\partial f_3}{\partial x} \\
&= 2\begin{bmatrix} \frac{\partial f_1}{\partial x} & \frac{\partial f_2}{\partial x} & \frac{\partial f_3}{\partial x} \end{bmatrix}^T \begin{bmatrix} f_1(x,y) \\ f_2(x,y) \\ f_3(x,y) \end{bmatrix}, \text{ and similarly:} \\
\frac{\partial r}{\partial y} &= 2\begin{bmatrix} \frac{\partial f_1}{\partial y} & \frac{\partial f_2}{\partial y} & \frac{\partial f_3}{\partial y} \end{bmatrix}^T \begin{bmatrix} f_1(x,y) \\ f_2(x,y) \\ f_3(x,y) \end{bmatrix}.
\end{aligned}$$

computing the gradient vector

We may divide by two as $\frac{\partial r}{\partial x} = 0$ and $\frac{\partial r}{\partial y} = 0$.

$$\frac{\partial r}{\partial x} = \begin{bmatrix} \frac{\partial f_1}{\partial x} & \frac{\partial f_2}{\partial x} & \frac{\partial f_3}{\partial x} \end{bmatrix}^T \begin{bmatrix} f_1(x,y) \\ f_2(x,y) \\ f_3(x,y) \end{bmatrix}$$

$$\frac{\partial r}{\partial y} = \begin{bmatrix} \frac{\partial f_1}{\partial y} & \frac{\partial f_2}{\partial y} & \frac{\partial f_3}{\partial y} \end{bmatrix}^T \begin{bmatrix} f_1(x,y) \\ f_2(x,y) \\ f_3(x,y) \end{bmatrix}$$

Then the gradient ∇r is

$$\nabla r = \begin{bmatrix} \frac{\partial f_1}{\partial x} & \frac{\partial f_2}{\partial x} & \frac{\partial f_3}{\partial x} \\ \frac{\partial f_1}{\partial y} & \frac{\partial f_2}{\partial y} & \frac{\partial f_3}{\partial y} \end{bmatrix} \begin{bmatrix} f_1(x,y) \\ f_2(x,y) \\ f_3(x,y) \end{bmatrix} = J_{\mathbf{f}}(x,y)^T \mathbf{f}(x,y).$$

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description of the method

Input: $\mathbf{f}(\mathbf{x}) = \mathbf{0}$, a system of m equations in n unknowns,
$\mathbf{x}_0$, an initial guess for a solution,
λ, value for the regularization parameter,
N, maximum number of iterations,
δ, tolerance on $||\Delta\mathbf{x}||$,
ϵ, tolerance on $||\mathbf{f}(\mathbf{x})||$.

for $k = 0, 1, \ldots, N$ do
  $\mathbf{r} := \mathbf{f}(\mathbf{x}_k)$
  $A := J_{\mathbf{f}}(\mathbf{x}_k)$
  solve $\left(A^T A + \lambda \text{diag}(A^T A)\right) \Delta\mathbf{x} = -A^T \mathbf{r}$
  $\mathbf{x}_{k+1} := \mathbf{x}_k + \Delta\mathbf{x}$
  exit when $(||\mathbf{r}|| \leq \epsilon)$ or $(||\Delta\mathbf{x}|| \leq \delta)$

define a Julia function

Exercise 4:

Use the pseudo code on the previous slide to define a function.

1. Document all parameters in `LevenbergMarquardt`, a Julia function for the method of Levenberg-Marquardt. Use good default values for N, δ, and ϵ.
2. Write the definition of your `LevenbergMarquardt`.
3. Illustrate the correctness of your function on the example of the near intersection points of three circles, using the default values for N, δ, and ϵ.
4. Experiment with $\lambda = 0, 10^{-2}, 1, 10^2, \ldots$. What is the best value for λ for the three circle problem?

a summary on least squares solving

What we covered in four lectures:

1. Solving a linear system in the least squares sense corresponds to constructing an orthogonal basis of the column space.

2. The classical Gram-Schmidt method loses orthogonality, the modified Gram-Schmidt method is numerically stable.

   The Householder QR method applies orthogonal transformations and is recommended for ill-conditioned inputs.

3. The Generalized Minimum Residual Method proceeds iteratively, solving smaller dimensional least squares problems in each step.

4. The method of Gauss-Newton updates the current approximation via the solution of a least squares system.

   Levenberg-Marquardt adds steepest descent to Gauss-Newton.