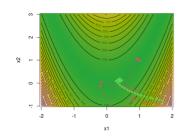
Optimization in Machine Learning

Second order methods Newton-Raphson



Learning goals

- Newton-Raphson
- Limitations



FROM FIRST TO SECOND ORDER METHODS

- So far: First order methods
 - ⇒ *Gradient* information, i.e., first derivatives
- Now: Second order methods
 - ⇒ *Hessian* information, i.e., second derivatives



NEWTON-RAPHSON

Assumption: $f \in C^2$

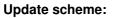
Aim: Find stationary point \mathbf{x}^* , i.e., $\nabla f(\mathbf{x}^*) = \mathbf{0}$

Idea: Find root of first order Taylor approximation of $\nabla f(\mathbf{x})$:

$$\nabla f(\mathbf{x}) \approx \nabla f(\mathbf{x}^{[t]}) + \nabla^2 f(\mathbf{x}^{[t]})(\mathbf{x} - \mathbf{x}^{[t]}) = \mathbf{0}$$

$$\nabla^2 f(\mathbf{x}^{[t]})(\mathbf{x} - \mathbf{x}^{[t]}) = -\nabla f(\mathbf{x}^{[t]})$$

$$\mathbf{x}^{[t+1]} = \mathbf{x}^{[t]} - (\nabla^2 f(\mathbf{x}^{[t]}))^{-1} \nabla f(\mathbf{x}^{[t]})$$



$$\mathbf{x}^{[t+1]} = \mathbf{x}^{[t]} + \mathbf{d}^{[t]}$$

with
$$\mathbf{d}^{[t]} = -\left(
abla^2 f(\mathbf{x}^{[t]}) \right)^{-1}
abla f(\mathbf{x}^{[t]})$$



NEWTON-RAPHSON / 2

Note: In practice, we get $\mathbf{d}^{[t]}$ by solving the linear system

$$\nabla^2 f(\mathbf{x}^{[t]}) \mathbf{d}^{[t]} = -\nabla f(\mathbf{x}^{[t]})$$

with direct (matrix decompositions) or iterative methods.

Relaxed/Damped Newton-Raphson: Use step size $\alpha > 0$ with

$$\mathbf{x}^{[t+1]} = \mathbf{x}^{[t]} + \alpha \mathbf{d}^{[t]}$$

to satisfy Wolfe conditions (or just Armijo rule)



ANALYTICAL EXAMPLE WITH QUADRATIC FORM

$$f(x_1,x_2)=x_1^2+\frac{x_2^2}{2}$$

Update direction: $\mathbf{d}^{[t]} = -\left(\nabla^2 f(x_1^{[t]}, x_2^{[t]})\right)^{-1} \nabla f(x_1^{[t]}, x_2^{[t]})$

$$\nabla f(x_1, x_2) = \begin{pmatrix} 2x_1 \\ x_2 \end{pmatrix}, \quad \nabla^2 f(x_1, x_2) = \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}$$

First step:

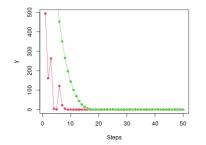
$$\begin{pmatrix} x_1^{[1]} \\ x_2^{[1]} \end{pmatrix} = \begin{pmatrix} x_1^{[0]} \\ x_2^{[0]} \end{pmatrix} + \mathbf{d}^{[0]} = \begin{pmatrix} x_1^{[0]} \\ x_2^{[0]} \end{pmatrix} - \begin{pmatrix} 1/2 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 2x_1^{[0]} \\ x_2^{[0]} \end{pmatrix}$$

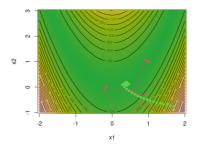
$$= \begin{pmatrix} x_1^{[0]} \\ x_2^{[0]} \end{pmatrix} + \begin{pmatrix} -x_1^{[0]} \\ -x_2^{[0]} \end{pmatrix} = \mathbf{0}$$

Note: Newton-Raphson only needs one iteration for quadratic forms



NEWTON-RAPHSON VS. GD ON BRANIN FUNCTION









DISCUSSION

Advantage:

• For *f* sufficiently smooth:

Newton-Raphson converges *locally* quadratically (i.e., for starting points close enough to stationary point)



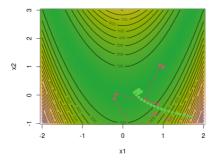
Disadvantage:

• For "bad" starting points:

Newton-Raphson may diverge

LIMITATIONS

Problem 1: In general, $\mathbf{d}^{[t]}$ is not a descent direction





But: If Hessian is positive definite, $\mathbf{d}^{[t]}$ is descent direction:

$$\nabla f(\boldsymbol{x}^{[t]})^{\top}\boldsymbol{d}^{[t]} = -\nabla f(\boldsymbol{x}^{[t]})^{\top} \left(\nabla^2 f(\boldsymbol{x}^{[t]})\right)^{-1} \nabla f(\boldsymbol{x}^{[t]}) < 0$$

Near minimum, Hessian is positive definite. For initial steps, Hessian is often not positive definite and Newton-Raphson may give non-descending update directions

LIMITATIONS / 2

Problem 2: Hessian can be **computationally expensive** to calculate, since descent direction $\mathbf{d}^{[t]}$ is the solution of the linear system

$$\nabla^2 f(\mathbf{x}^{[t]}) \mathbf{d}^{[t]} = -\nabla f(\mathbf{x}^{[t]}).$$



- Quasi-Newton method
- Gauss-Newton algorithm (for least squares)

