#### ECE276A: Sensing & Estimation in Robotics Lecture 4: Unconstrained Optimization

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# Unconstrained Optimization

Many problems we encounter in this course, lead to an unconstrained optimization problem over the Euclidean vector space R<sup>d</sup>:

$$\min_{\mathbf{x}\in\mathbb{R}^d}f(\mathbf{x})$$

- ▶ A global minimizer  $\mathbf{x}^* \in \mathbb{R}^d$  satisfies  $f(\mathbf{x}^*) \leq f(\mathbf{x})$  for all  $\mathbf{x} \in \mathbb{R}^d$ . The value  $f(\mathbf{x}^*)$  is called global minimum.
- ▶ A local minimizer  $\mathbf{x}^* \in \mathbb{R}^d$  satisfies  $f(\mathbf{x}^*) \leq f(\mathbf{x})$  for all  $\mathbf{x} \in \mathcal{N}(\mathbf{x}^*)$ , where  $\mathcal{N}(\mathbf{x}^*) \subset \mathbb{R}^d$  is a neighborhood around  $\mathbf{x}^*$  (e.g., an open ball with small radius centered at  $\mathbf{x}^*$ ). The value  $f(\mathbf{x}^*)$  is called local minimum.
- The objective function  $f : \mathbb{R}^d \mapsto \mathbb{R}$  is **differentiable** if the gradient:

$$abla f(\mathbf{x}) := \begin{bmatrix} rac{\partial f(\mathbf{x})}{\partial x_1} & \cdots & rac{\partial f(\mathbf{x})}{\partial x_d} \end{bmatrix}^{ op} \in \mathbb{R}^d$$

exists at each  $\mathbf{x} \in \mathbb{R}^d$ 

A critical point x

 € ℝ<sup>d</sup> satisfies ∇f(x
 ) = 0 or ∇f(x
 ) = undefined

 All minimizers are critical points but not all critical points are
 minimizers. A critical point is either a local maximizer, a local
 minimizer, or neither (saddle point).

Convexity

▶ A set  $\mathcal{D} \subseteq \mathbb{R}^d$  is convex if  $\lambda \mathbf{x} + (1 - \lambda)\mathbf{y} \in \mathcal{D}$  for all  $\mathbf{x}, \mathbf{y} \in \mathcal{D}$ ,  $\lambda \in [0, 1]$ 

A convex set contains the line segment between any two points in it Convex set
Non - convex set



- A function  $f : \mathcal{D} \mapsto \mathbb{R}$  with  $\mathcal{D} \subseteq \mathbb{R}^d$  is **convex** if:
  - D is a convex set
  - ►  $f(\lambda \mathbf{x} + (1 \lambda)\mathbf{y}) \le \lambda f(\mathbf{x}) + (1 \lambda)f(\mathbf{y})$  for all  $\mathbf{x}, \mathbf{y} \in \mathcal{D}$ ,  $\lambda \in [0, 1]$
- First-order convexity condition: a differentiable  $f : \mathcal{D} \mapsto \mathbb{R}$  with convex  $\mathcal{D}$  is convex iff  $f(\mathbf{y}) \ge f(\mathbf{x}) + \nabla f(\mathbf{x})^{\top} (\mathbf{y} \mathbf{x})$  for all  $\mathbf{x}, \mathbf{y} \in \mathcal{D}$
- Second-order convexity condition: a twice-differentiable f : D → ℝ with convex D is convex iff ∇<sup>2</sup>f(x) ≥ 0 for all x ∈ D

# Descent Direction

Consider the **unconstrained optimization problem**:

 $\min_{\mathbf{x}\in\mathbb{R}^d}f(\mathbf{x})$ 

#### Descent Direction Theorem

Suppose f is differentiable at  $\bar{\mathbf{x}}$ . If  $\exists \delta \mathbf{x}$  such that  $\nabla f(\bar{\mathbf{x}})^{\top} \delta \mathbf{x} < 0$ , then  $\exists \epsilon > 0$  such that  $f(\bar{\mathbf{x}} + \alpha \delta \mathbf{x}) < f(\bar{\mathbf{x}})$  for all  $\alpha \in (0, \epsilon)$ .

- The vector  $\delta \mathbf{x}$  is called a **descent direction**
- The theorem states that if a descent direction exists at x
  , then it is possible to move to a new point that has a lower f value
- Steepest descent direction:  $\delta \mathbf{x} := -\frac{\nabla f(\bar{\mathbf{x}})}{\|\nabla f(\bar{\mathbf{x}})\|}$
- Based on this theorem, we can derive conditions for determining the optimality of x

# **Optimality Conditions**

#### First-order Necessary Condition

Suppose f is differentiable at  $\bar{\mathbf{x}}$ . If  $\bar{\mathbf{x}}$  is a local minimizer, then  $\nabla f(\bar{\mathbf{x}}) = 0$ .

#### Second-order Necessary Condition

Suppose f is twice-differentiable at  $\bar{\mathbf{x}}$ . If  $\bar{\mathbf{x}}$  is a local minimizer, then  $\nabla f(\bar{\mathbf{x}}) = 0$  and  $\nabla^2 f(\bar{\mathbf{x}}) \succeq 0$ .

#### Second-order Sufficient Condition

Suppose f is twice-differentiable at  $\bar{\mathbf{x}}$ . If  $\nabla f(\bar{\mathbf{x}}) = 0$  and  $\nabla^2 f(\bar{\mathbf{x}}) \succ 0$ , then  $\bar{\mathbf{x}}$  is a local minimizer.

#### Necessary and Sufficient Condition

Suppose f is differentiable at  $\bar{\mathbf{x}}$ . If f is **convex**, then  $\bar{\mathbf{x}}$  is a global minimizer **if and only if**  $\nabla f(\bar{\mathbf{x}}) = 0$ .

## Descent Optimization Methods

- A critical point of f can be obtained by solving ∇f(x) = 0 but an explicit solution may be difficult to derive
- **Descent methods**: iterative methods to obtain a solution of  $\nabla f(\mathbf{x}) = 0$
- Given an initial guess x<sup>(k)</sup>, take a step of size α<sup>(k)</sup> > 0 along a descent direction δx<sup>(k)</sup>:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha^{(k)} \delta \mathbf{x}^{(k)}$$

- ▶ Different methods differ in the way  $\delta \mathbf{x}^{(k)}$  and  $\alpha^{(k)}$  are chosen
- $\delta \mathbf{x}^{(k)}$  needs to be a descent direction:  $\nabla f(\mathbf{x}^{(k)})^{\top} \delta \mathbf{x}^{(k)} < 0, \forall \mathbf{x}^{(k)} \neq \mathbf{x}^{*}$

▶ In practice,  $\alpha^{(k)}$  is obtained via approximate line search methods

Gradient Descent (First-Order Method)

▶ Idea:  $-\nabla f(\mathbf{x}^{(k)})$  points in the direction of steepest local descent

• Gradient descent: let  $\delta \mathbf{x}^{(k)} := -\nabla f(\mathbf{x}^{(k)})$  and iterate:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha^{(k)} \nabla f(\mathbf{x}^{(k)})$$

Step size: a good choice for α<sup>(k)</sup> is <sup>1</sup>/<sub>L</sub>, where L > 0 is the Lipschitz constant of ∇f(x):

$$\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{x}')\| \le L \|\mathbf{x} - \mathbf{x}'\| \qquad \forall \mathbf{x}, \mathbf{x}' \in \mathbb{R}^d$$

# Newton's Method (Second-Order Method)

- ▶ Newton's method: iteratively approximates f by a quadratic function
- Since δx is a 'small' change to the initial guess x<sup>(k)</sup>, we can approximate f using a Taylor-series expansion:



► The symmetric Hessian matrix ∇<sup>2</sup>f(x<sup>(k)</sup>) needs to be positive-definite for this method to work.

#### Newton's Method (Second-Order Method)



# Newton's Method (Second-Order Method)

- Find  $\delta \mathbf{x}$  that minimizes the quadratic approximation to  $f(\mathbf{x}^{(k)} + \delta \mathbf{x})$
- Since this is an unconstrained optimization problem, δx can be determined by setting the derivative with respect to δx to zero:

$$0 = \frac{\partial q(\delta \mathbf{x}, \mathbf{x}^{(k)})}{\partial \delta \mathbf{x}} = \left( \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \Big|_{\mathbf{x} = \mathbf{x}^{(k)}} \right) + \delta \mathbf{x}^{\top} \left( \frac{\partial^2 f(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^{\top}} \Big|_{\mathbf{x} = \mathbf{x}^{(k)}} \right)$$
$$\Rightarrow \quad \left( \frac{\partial^2 f(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^{\top}} \Big|_{\mathbf{x} = \mathbf{x}^{(k)}} \right) \delta \mathbf{x} = - \left( \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \Big|_{\mathbf{x} = \mathbf{x}^{(k)}} \right)^{\top}$$

The above is a linear system of equations and can be solved when the Hessian is invertible, i.e., ∇<sup>2</sup>f(x<sup>(k)</sup>) ≻ 0:

$$\delta \mathbf{x} = -\left[\nabla^2 f(\mathbf{x}^{(k)})\right]^{-1} \nabla f(\mathbf{x}^{(k)})$$

Newton's method:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha^{(k)} \left[ \nabla^2 f(\mathbf{x}^{(k)}) \right]^{-1} \nabla f(\mathbf{x}^{(k)})$$

# Newton's Method (Comments)

- Newton's method, like any other descent method, converges only to a local minimum
- Damped Newton phase: when the iterates are "far away" from the optimal point, the function value is decreased sublinearly, i.e., the step sizes α<sup>(k)</sup> are small
- Quadratic convergence phase: when the iterates are "sufficiently close" to the optimum, full Newton steps are taken, i.e.,  $\alpha^{(k)} = 1$ , and the function value converges quadratically to the optimum
- A disadvantage of Newton's method is the need to form the Hessian, which can be numerically ill-conditioned or very computationally expensive in high-dimensional problems

### Gauss-Newton's Method

Gauss-Newton is an approximation to Newton's method that avoids computing the Hessian. It is applicable when the objective function has the following quadratic form:

$$f(\mathbf{x}) = rac{1}{2} \mathbf{e}(\mathbf{x})^{ op} \mathbf{e}(\mathbf{x}) \qquad \mathbf{e}(\mathbf{x}) \in \mathbb{R}^m$$

The Jacobian and Hessian matrices are:

Jacobian: 
$$\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}} = \mathbf{e}(\mathbf{x}^{(k)})^{\top} \left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right)$$
  
Hessian: 
$$\frac{\partial^2 f(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^{\top}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}} = \left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right)^{\top} \left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right)$$
$$+ \sum_{i=1}^{m} e_i(\mathbf{x}^{(k)}) \left(\frac{\partial^2 e_i(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^{\top}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right)$$

### Gauss-Newton's Method

Near the minimum of f, the second term in the Hessian is small relative to the first and the Hessian can be approximated according to:

$$\frac{\partial^2 f(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}^{\top}} \bigg|_{\mathbf{x} = \mathbf{x}^{(k)}} \approx \left( \frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}} \bigg|_{\mathbf{x} = \mathbf{x}^{(k)}} \right)^{\top} \left( \frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}} \bigg|_{\mathbf{x} = \mathbf{x}^{(k)}} \right)$$

The above does not involve any second derivatives

Setting the gradient of this new quadratic approximation of *f* with respect to δx to zero, leads to the system:

$$\left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right)^{\top} \left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right) \delta \mathbf{x} = -\left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right)^{\top} \mathbf{e}(\mathbf{x}^{(k)})$$

Gauss-Newton's method:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha^{(k)} \delta \mathbf{x}$$

# Gauss-Newton's Method (Alternative Derivation)

Another way to think about the Gauss-Newton method is to start with a Taylor expansion of e(x) instead of f(x):

$$\mathbf{e}(\mathbf{x}^{(k)} + \delta \mathbf{x}) \approx \mathbf{e}(\mathbf{x}^{(k)}) + \left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x} = \mathbf{x}^{(k)}}\right) \delta \mathbf{x}$$

Substituting into f leads to:

$$f(\mathbf{x}^{(k)} + \delta \mathbf{x}) \approx \frac{1}{2} \left( \mathbf{e}(\mathbf{x}^{(k)}) + \left( \frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}} \Big|_{\mathbf{x} = \mathbf{x}^{(k)}} \right) \delta \mathbf{x} \right)^{\top} \left( \mathbf{e}(\mathbf{x}^{(k)}) + \left( \frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}} \Big|_{\mathbf{x} = \mathbf{x}^{(k)}} \right) \delta \mathbf{x} \right)$$

• Minimizing this with respect to  $\delta x$  leads to the same system as before:

$$\left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right)^{\top} \left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right) \delta \mathbf{x} = -\left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right)^{\top} \mathbf{e}(\mathbf{x}^{(k)})$$

## Levenberg-Marquardt's Method

The Levenberg-Marquardt modification to the Gauss-Newton method uses a positive diagonal matrix D to condition the Hessian approximation:

$$\left(\left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right)^{\top} \left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right) + \lambda D\right) \delta \mathbf{x} = -\left(\frac{\partial \mathbf{e}(\mathbf{x})}{\partial \mathbf{x}}\Big|_{\mathbf{x}=\mathbf{x}^{(k)}}\right)^{\top} \mathbf{e}(\mathbf{x}^{(k)})$$

When λ ≥ 0 is large, the descent vector δx corresponds to a very small step in the direction of steepest descent. This helps when the Hessian approximation is poor or poorly conditioned by providing a meaningful direction.

# Levenberg-Marquardt's Method (Summary)

An iterative optimization approach for the unconstrained problem:

$$\min_{\mathbf{x}} f(\mathbf{x}) := \frac{1}{2} \sum_{j} \mathbf{e}_{j}(\mathbf{x})^{\top} \mathbf{e}_{j}(\mathbf{x}) \qquad \mathbf{e}_{j}(\mathbf{x}) \in \mathbb{R}^{m_{j}}, \ \mathbf{x} \in \mathbb{R}^{n}$$

• Given an initial guess  $\mathbf{x}^{(k)}$ , determine a descent direction  $\delta \mathbf{x}$  by solving:

$$\left(\sum_{j} J_j(\mathbf{x}^{(k)})^\top J_j(\mathbf{x}^{(k)}) + \lambda D\right) \delta \mathbf{x} = -\left(\sum_{j} J_j(\mathbf{x}^{(k)})^\top \mathbf{e}_j(\mathbf{x}^{(k)})\right)$$

where  $J_j(\mathbf{x}) := \frac{\partial \mathbf{e}_j(\mathbf{x})}{\partial \mathbf{x}} \in \mathbb{R}^{m_j \times n}$ ,  $\lambda \ge 0$ ,  $D \in \mathbb{R}^{n \times n}$  is a positive diagonal matrix, e.g.,  $D = \operatorname{diag}\left(\sum_j J_j(\mathbf{x}^{(k)})^\top J_j(\mathbf{x}^{(k)})\right)$ 

Obtain an updated estimate according to:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha^{(k)} \delta \mathbf{x}$$

# Unconstrained Optimization Example

• Let  $f(\mathbf{x}) := \frac{1}{2} \sum_{j=1}^{n} \|A_j \mathbf{x} + b_j\|_2^2$  for  $\mathbf{x} \in \mathbb{R}^d$  and assume  $\sum_{j=1}^{n} A_j^\top A_j \succ 0$ 

Solve the unconstrained optimization problem min<sub>x</sub> f(x) using:

- The necessary and sufficient optimality condition for convex function f
- Gradient descent
- Newton's method
- Gauss-Newton's method

• We will need  $\nabla f(\mathbf{x})$  and  $\nabla^2 f(\mathbf{x})$ :

$$\frac{df(\mathbf{x})}{d\mathbf{x}} = \frac{1}{2} \sum_{j=1}^{n} \frac{d}{d\mathbf{x}} ||A_j \mathbf{x} + b_j||_2^2 = \sum_{j=1}^{n} (A_j \mathbf{x} + b_j)^\top A_j$$
$$\nabla f(\mathbf{x}) = \frac{df(\mathbf{x})}{d\mathbf{x}}^\top = \left(\sum_{j=1}^{n} A_j^\top A_j\right) \mathbf{x} + \left(\sum_{j=1}^{n} A_j^\top b_j\right)$$
$$\nabla^2 f(\mathbf{x}) = \frac{d}{d\mathbf{x}} \nabla f(\mathbf{x}) = \sum_{j=1}^{n} A_j^\top A_j \succ 0$$

Necessary and Sufficient Optimality Condition

Solve  $\nabla f(\mathbf{x}) = 0$  for  $\mathbf{x}$ :

$$0 = \nabla f(\mathbf{x}) = \left(\sum_{j=1}^{n} A_j^{\top} A_j\right) \mathbf{x} + \left(\sum_{j=1}^{n} A_j^{\top} b_j\right)$$
$$\mathbf{x} = -\left(\sum_{j=1}^{n} A_j^{\top} A_j\right)^{-1} \left(\sum_{j=1}^{n} A_j^{\top} b_j\right)$$

▶ The solution above is unique since we assumed that  $\sum_{j=1}^{n} A_j^{\top} A_j \succ 0$ 

# Gradient Descent

Start with an initial guess x<sup>(0)</sup> = 0

- At iteration k, gradient descent uses the descent direction δ**x**<sup>(k)</sup> = -∇f(**x**<sup>(k)</sup>)
- Given arbitary  $\mathbf{x}_1, \mathbf{x}_2 \in \mathbb{R}^d$ , determine the Lipschitz constant of  $\nabla f(\mathbf{x})$ :

$$\|\nabla f(\mathbf{x}_1) - \nabla f(\mathbf{x}_2)\| = \left\| \left( \sum_{j=1}^n A_j^\top A_j \right) (\mathbf{x}_1 - \mathbf{x}_2) \right\| \le \underbrace{\left\| \sum_{j=1}^n A_j^\top A_j \right\|}_{L} \|\mathbf{x}_1 - \mathbf{x}_2\|$$

• Choose step size  $\alpha^{(k)} = \frac{1}{L}$  and iterate:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha^{(k)} \delta \mathbf{x}^{(k)}$$
$$= \mathbf{x}^{(k)} - \frac{1}{L} \left( \sum_{j=1}^{n} A_j^{\top} A_j \right) \mathbf{x}^{(k)} - \frac{1}{L} \left( \sum_{j=1}^{n} A_j^{\top} b_j \right)$$

# Newton's Method

• Start with an initial guess  $\mathbf{x}^{(0)} = \mathbf{0}$ 

At iteration k, Newton's method uses the descent direction:

$$\delta \mathbf{x}^{(k)} = -\left[\nabla^2 f(\mathbf{x}^{(k)})\right]^{-1} \nabla f(\mathbf{x}^{(k)})$$
$$= -\mathbf{x}^{(k)} - \left(\sum_{j=1}^n A_j^\top A_j\right)^{-1} \left(\sum_{j=1}^n A_j^\top b_j\right)$$

and updates the solution estimate via:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \delta \mathbf{x}^{(k)} = -\left(\sum_{j=1}^{n} A_j^{\top} A_j\right)^{-1} \left(\sum_{j=1}^{n} A_j^{\top} b_j\right)$$

Note that for this problem, Newton's method converges in one iteration!

### Gauss-Newton's Method

- ►  $f(\mathbf{x})$  is of the form  $\frac{1}{2} \sum_{j=1}^{n} \mathbf{e}_j(\mathbf{x})^\top \mathbf{e}_j(\mathbf{x})$  for  $\mathbf{e}_j(\mathbf{x}) := A_j \mathbf{x} + b_j$
- The Jacobian of  $\mathbf{e}_j(\mathbf{x})$  is  $J_j(\mathbf{x}) = A_j$
- Start with an initial guess  $\mathbf{x}^{(0)} = \mathbf{0}$
- ▶ At iteration k, Gauss-Newton's method uses the descent direction:

$$\delta \mathbf{x}^{(k)} = -\left(\sum_{j=1}^{n} J_j(\mathbf{x}^{(k)})^{\top} J_j(\mathbf{x}^{(k)})\right)^{-1} \left(\sum_{j=1}^{n} J_j(\mathbf{x}^{(k)})^{\top} \mathbf{e}_j(\mathbf{x}^{(k)})\right)$$
$$= -\left(\sum_{j=1}^{n} A_j^{\top} A_j\right)^{-1} \left(\sum_{j=1}^{n} A_j^{\top} (A_j \mathbf{x}^{(k)} + b_j)\right)$$
$$= -\mathbf{x}^{(k)} - \left(\sum_{j=1}^{n} A_j^{\top} A_j\right)^{-1} \left(\sum_{j=1}^{n} A_j^{\top} b_j\right)$$

If α<sup>(k)</sup> = 1, in this problem, Gauss-Newton's method behaves exactly like Newton's method and coverges in one iteration!

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