## Purpose:

How to train an MLP neural network in MATLAB environment!

## that is

> For good computations, $\frac{\text { we need good formulae }}{\text { for good algorithms; }}$ and good visualization for good illustration and proper testing of good methods and succesfull applications!

## Critical values:




## Theoretical bases of optimization problems:

$$
\text { Minimize } \quad \mathcal{J}(\mathbf{u}) \quad \text { where } \mathbf{u}=\left[\begin{array}{c}
u_{1}  \tag{1}\\
\vdots \\
u_{n}
\end{array}\right] \in \mathbf{R}^{n} .
$$

- $\mathcal{J}: \mathbf{R}^{n} \rightarrow \mathbf{R}$ cost function(al) measuring the goodness of a solution candidate:

NOTICE: good measure $\Rightarrow$ good problem $\Rightarrow$ useful solution $(A \Rightarrow B \equiv \neg B \rightarrow \neg A$ !)

- we assume that $\mathcal{J}(\mathbf{u}) \geq 0 \quad \forall \mathbf{u} \in \mathbf{R}^{n}$
- NOTICE: $\max _{\mathbf{u}} \mathcal{J}(\mathbf{u}) \equiv \min _{\mathbf{u}}-\mathcal{J}(\mathbf{u})$
- we are seeking the values of $\left(u_{1}, \ldots, u_{n}\right)$ (unknowns)
- through the following definitions we introduce precise characterization of the visual intuition of the previous (and the following) figures

Definition 1. Vector $\mathbf{u}^{*}$ is the (strict) global minimum of problem (1) if

$$
\mathcal{J}\left(\mathbf{u}^{*}\right) \leq(<) \mathcal{J}(\mathbf{u}) \quad \text { for all } \mathbf{u} \in \mathbf{R}^{n}
$$

Definition 2. Vector $\mathbf{u}^{*}$ is the (strict) local minimum of problem (1) if there exists a $\delta>0$ such that

$$
\mathcal{J}\left(\mathbf{u}^{*}\right) \leq(<) \mathcal{J}(\mathbf{u}), \quad \text { for all } \mathbf{u} \in \mathbf{R}^{n} \text { such that }\left\|\mathbf{u}-\mathbf{u}^{*}\right\| \leq \delta
$$

Theorem 1. (Weierstraas) If function $\mathcal{J}$ in problem (1) is continuous, then there exists a minimum solution $\mathbf{u}^{*}$.
Definition 3. Function $\mathcal{J}$ is convex if

$$
\mathcal{J}(\lambda \mathbf{x}+(1-\lambda) \mathbf{y}) \leq \lambda \mathcal{J}(\mathbf{x})+(1-\lambda) \mathcal{J}(\mathbf{y}) \quad \forall \mathbf{x}, \mathbf{y} \in \mathbf{R}^{n} \text { and } 0 \leq \lambda \leq 1
$$

Strict convexity requires $<$ instead of $\leq$ for $\mathbf{x} \neq \mathbf{y}$.
Theorem 2. For (locally) convex (and bounded from below) function $\mathcal{J}$ there exists a (local) minimum. If $\mathcal{J}$ is (locally) strictly convex, then the minimum point is (locally) unique.

## Theoretical bases of gradient methods:



1D mean value theorem of differential calculus:

$$
f(x)=f(y)+f^{\prime}(\xi)(x-y) \quad \text { for some } \xi \in(y, x)
$$

- through the following definitions we generalize both the concept of derivative and its relation to local function approximation in 1D into higher-order spaces


## Theoretical bases of gradient methods II:

Definition 4. Function $\mathcal{J}$ is (continuously) differentiable at $\mathbf{u}\left(\mathcal{J} \in C^{1}\left(\mathbf{R}^{n}\right)\right.$ ), if there exists vector $\nabla \mathcal{J}(\mathbf{u}) \in \mathbf{R}^{n}$ and function $\varepsilon: \mathbf{R}^{n} \rightarrow \mathbf{R}$ such that

$$
\begin{equation*}
\mathcal{J}(\overline{\mathbf{u}})=\mathcal{J}(\mathbf{u})+\nabla \mathcal{J}(\mathbf{u})^{T}(\overline{\mathbf{u}}-\mathbf{u})+\|\overline{\mathbf{u}}-\mathbf{u}\| \varepsilon(\mathbf{u}, \overline{\mathbf{u}}-\mathbf{u}) \tag{2}
\end{equation*}
$$

for all $\overline{\mathbf{u}} \in \mathbf{R}^{n}$ and $\varepsilon(\mathbf{u}, \overline{\mathbf{u}}-\mathbf{u}) \rightarrow 0$ when $\overline{\mathbf{u}} \rightarrow \mathbf{u}$.
Vector $\nabla \mathcal{J}(\mathbf{u})$ is the gradient of $\mathcal{J}$ at $\mathbf{u}$ consisting of the partial derivatives:

$$
\nabla \mathcal{J}(\mathbf{u})=\left[\begin{array}{c}
\frac{\partial \mathcal{J}(\mathbf{u})}{\partial u_{1}}  \tag{3}\\
\vdots \\
\frac{\partial \mathcal{J}(\mathbf{u})}{\partial u_{n}}
\end{array}\right] \simeq\left[\begin{array}{c}
\frac{\partial}{\partial u_{1}} \\
\vdots \\
\frac{\partial}{\partial u_{n}}
\end{array}\right] \mathcal{J}(\mathbf{u}) .
$$

Definition 5. Function $\mathcal{J}$ is twice (continuously) differentiable at $\mathbf{u}\left(\mathcal{J} \in C^{2}\left(\mathbf{R}^{n}\right)\right.$ ), if there exists vector $\nabla \mathcal{J}(\mathbf{u}) \in \mathbf{R}^{n}$ and symmetric $n \times n$-matrix $\mathbf{H}(\mathbf{u})$, the so-called Hessian matrix, and function $\varepsilon: \mathbf{R}^{n} \rightarrow \mathbf{R}$ such that

$$
\begin{equation*}
\mathcal{J}(\overline{\mathbf{u}})=\mathcal{J}(\mathbf{u})+\nabla \mathcal{J}(\mathbf{u})^{T}(\overline{\mathbf{u}}-\mathbf{u})+\frac{1}{2}(\overline{\mathbf{u}}-\mathbf{u})^{T} \mathbf{H}(\mathbf{u})(\overline{\mathbf{u}}-\mathbf{u})+\|\overline{\mathbf{u}}-\mathbf{u}\|^{2} \varepsilon(\mathbf{u}, \overline{\mathbf{u}}-\mathbf{u}) \tag{4}
\end{equation*}
$$

where (again) $\varepsilon(\mathbf{u}, \overline{\mathbf{u}}-\mathbf{u}) \rightarrow 0$ when $\overline{\mathbf{u}} \rightarrow \mathbf{u}$.
Hessian matrix consists of the second-order partial derivatives $\frac{\partial^{2} \mathcal{J}(\mathbf{u})}{\partial u_{i} \partial u_{j}}$ :

$$
\mathbf{H}(\mathbf{u})\left(\simeq \nabla\left(\nabla^{T} \mathcal{J}(\mathbf{u})\right) \simeq \nabla^{2} \mathcal{J}(\mathbf{u})\right)=\left[\begin{array}{ccc}
\frac{\partial^{2} \mathcal{J}(\mathbf{u})}{\partial u_{1}^{2}} & \ldots & \frac{\partial^{2} \mathcal{J}(\mathbf{u})}{\partial u_{1} \partial u_{n}} \\
\vdots & \ddots & \vdots \\
\frac{\partial^{2} \mathcal{J}(\mathbf{u})}{\partial u_{n} \partial u_{1}} & \ldots & \frac{\partial^{2} \mathcal{J}(\mathbf{u})}{\partial u_{n}^{2}}
\end{array}\right]
$$

Definition 6. Vector $\mathbf{d} \in \mathbf{R}^{n}$ is descent direction for function $\mathcal{J}$ at $\overline{\mathbf{u}}$, if there exists $\delta>0$ such that

$$
\mathcal{J}(\overline{\mathbf{u}}+t \mathbf{d})<\mathcal{J}(\overline{\mathbf{u}}) \quad \text { for all } t \in(0, \delta]
$$

Definition 7. Let $\mathcal{J}$ be differentiable at $\overline{\mathbf{u}}$. If there exists a direction $\mathbf{d} \in \mathbf{R}^{n}$ such that $\nabla \mathcal{J}(\overline{\mathbf{u}})^{T} \mathbf{d}<0$, then $\mathbf{d}$ is descent direction for $\mathcal{J}$ at $\overline{\mathbf{u}}$.
Theorem 3. Let $\mathcal{J}$ be differentiable at $\mathbf{u}^{*}$. If $\mathbf{u}^{*}$ is local minimum, then $\nabla \mathcal{J}\left(\mathbf{u}^{*}\right)=0$ (i.e., $\mathbf{u}^{*}$ is a critical value of $\left.\mathcal{J}\right)$.
Theorem 4. Let $\mathcal{J}$ be twice differentiable at $\mathbf{u}^{*}$. If $\mathbf{u}^{*}$ is local minimum, then $\nabla \mathcal{J}\left(\mathbf{u}^{*}\right)=0$ and the Hessian matrix $\mathbf{H}\left(\mathbf{u}^{*}\right)$ is positive semidefinite. If $\nabla \mathcal{J}\left(\mathbf{u}^{*}\right)=0$ and $\mathbf{H}\left(\mathbf{u}^{*}\right)$ is positive definite, then $\mathbf{u}^{*}$ is strict local minimum.

## Two examples:

As an example, we consider a few least-mean-squares (LMS) (quadratic) cost functionals and the corresponding optimization problems. Let $\left\{\mathrm{x}_{1}, \ldots, \mathrm{x}_{N}\right\}$ be a given set of (random) vectors such that $\mathbf{x}_{i} \in \mathbf{R}^{n}$ for all $1 \leq i \leq N$.
i) Mean:

$$
\mathcal{J}(\mathbf{u})=\sum_{i=1}^{N} \frac{1}{2}\left\|\mathbf{u}-\mathbf{x}_{i}\right\|^{2}=\sum_{i=1}^{N} \frac{1}{2}\left(\mathbf{u}-\mathbf{x}_{i}\right)^{T}\left(\mathbf{u}-\mathbf{x}_{i}\right)=\sum_{i=1}^{N} \frac{1}{2}\left(\sum_{j=1}^{n}\left(u_{j}-\left(\mathbf{x}_{i}\right)_{j}\right)^{2}\right) .
$$

Because $\frac{1}{2} \frac{\partial\left(u_{j}-\left(\mathbf{x}_{i_{j}}\right)^{2}\right.}{\partial u_{j}}=\left(\mathbf{u}-\mathbf{x}_{i}\right)_{j}$ for all $i, j$, we obtain

$$
\nabla \mathcal{J}(\mathbf{u})=\sum_{i=1}^{N}\left(\mathbf{u}-\mathbf{x}_{i}\right)=N \mathbf{u}-\sum_{i=1}^{N} \mathbf{x}_{i}
$$

When $\mathbf{u}$ is solved from $\nabla \mathcal{J}\left(\mathbf{u}^{*}\right)=0$, we get the sample mean

$$
\mathbf{u}^{*}=\frac{1}{N} \sum_{i=1}^{N} \mathbf{x}_{i}=\overline{\mathbf{x}}
$$

Notice that if there is some (measurement, quantization) error like $\mathbf{x}_{i}=\tilde{\mathbf{x}}_{i}+\varepsilon_{i}$, then $\mathbf{u}^{*}=\frac{1}{N} \sum_{i=1}^{N} \tilde{\mathbf{x}}_{i}+\frac{1}{N} \sum_{i=1}^{N} \varepsilon_{i}$. Hence, when $N \rightarrow \infty$ or $\varepsilon_{i} \in \mathcal{N}\left(0, \delta^{2}\right)$ (in general, any symmetric error distribution with "enough samples"), $\mathbf{u}^{*}$ is a good estimate for the average behaviour of the given sample.
Finally, $\mathbf{H}\left(\mathbf{u}^{*}\right)=\nabla^{T}(\nabla \mathcal{J}(u))=N \mathbf{I}$, so that $\overline{\mathbf{x}}$ is always unique.
ii) Linear fit: let $n=2$ and

$$
\mathcal{J}(\mathbf{u})=\frac{1}{2} \sum_{i=1}^{N}\left|\left(\mathbf{x}_{i}\right)_{2}-\left(u_{2}\left(\mathbf{x}_{i}\right)_{1}+u_{1}\right)\right|^{2}
$$

Then

$$
\begin{aligned}
& \frac{\partial \mathcal{J}(\mathbf{u})}{\partial u_{1}}=-\sum_{i=1}^{N}\left(\left(\mathbf{x}_{i}\right)_{2}-\left(u_{2}\left(\mathbf{x}_{i}\right)_{1}+u_{1}\right)\right) \\
& \frac{\partial \mathcal{J}(\mathbf{u})}{\partial u_{2}}=-\sum_{i=1}^{N}\left(\left(\mathbf{x}_{i}\right)_{2}-\left(u_{2}\left(\mathbf{x}_{i}\right)_{1}+u_{1}\right)\right)\left(\mathbf{x}_{i}\right)_{1}
\end{aligned}
$$

and

$$
\mathbf{H}(\mathbf{u})=\left[\begin{array}{cc}
N & \sum_{i=1}^{N}\left(\mathbf{x}_{i}\right)_{1} \\
\sum_{i=1}^{N}\left(\mathbf{x}_{i}\right)_{1} & \sum_{i=1}^{N}\left(\mathbf{x}_{i}\right)_{1}^{2}
\end{array}\right] \quad \text { Error in lecture notes!!!. }
$$

## Basic Algorithm:

1. Choose a starting point $\mathbf{u}^{0}$. Set iteration counter $k=0$.
2. Generate a descent direction $\mathbf{d}^{k}$.
3. Generate a step length $t^{k}$ such that $\mathcal{J}\left(\mathbf{u}^{k}+t^{k} \mathbf{d}^{k}\right)<\mathcal{J}\left(\mathbf{u}^{k}\right)$.
4. Update $\mathbf{u}^{k+1}=\mathbf{u}^{k}+t^{k} \mathbf{d}^{k}$.
5. Stopping test. If need to continue, set $k=k+1$ and go to 2 .

## When to Stop?

For chosen $\varepsilon>0$ :

- (Absolute) critical point: $\left\|\nabla \mathcal{J}\left(\mathbf{u}^{k+1}\right)\right\| \leq \varepsilon$.
- (Relative) critical point: $\left\|\nabla \mathcal{J}\left(\mathbf{u}^{k+1}\right)\right\| \leq \varepsilon\left\|\nabla \mathcal{J}\left(\mathbf{u}^{0}\right)\right\|$.
- Change of solution: $\left\|\mathbf{u}^{k+1}-\mathbf{u}^{k}\right\|=t^{k}\left\|\mathbf{d}^{k}\right\| \leq \varepsilon$.
- (Relative) change of cost functional:
$\frac{\mathcal{J}\left(u^{k+1}\right)-\mathcal{J}\left(\mathbf{u}^{k}\right)}{\max \left(\delta,\left|\mathcal{J}\left(\mathbf{u}^{k}\right)\right|, \mid \mathcal{J}\left(\mathbf{u}^{k+1} \mid\right)\right.} \leq \varepsilon, \quad$ where $\delta>0$.


## Qualities of a good algorithm?

1. convergence (it solves the problem...)
2. speed of convergence (fastly...)
3. memory efficiency (with low memory consumption; usually contradicts 2 .)

## Stepsize determination:

- assume that a descent direction $\mathbf{d}^{k}$ is given
- we review different possibilities for selecting $t^{k}$ appropriately
- starting point is to consider the following 1D minimization problem

$$
\begin{equation*}
\min _{t \in I} \mathcal{J}\left(\mathbf{u}^{k}+t \mathbf{d}^{k}\right)=j(t), \tag{5}
\end{equation*}
$$

where $I$ is a priori given search interval, usually $I=[0,1]$ (cf. Definition 3 of convexity)

- in principle, any minimization method for (5) is sufficient (halfing method(?), regulafalsi, golden search, etc.), but one must try to cope with previous quality attributes of a good overall method
$\Rightarrow \underline{\text { compromise: compute quickly "good enough" solution for (5)! }}$


## Basic approaches:

- Fixed stepsize: choose by hand some stepsize $0<t^{*}<1$ and use it throughout the optimization iterations. Convergence questionable and slow, usual values, e.g. $t^{*}=$ $0.01,0.05,0.1$.
- Armijo-rule: Search smaller stepsizes consequtively by testing the sufficient decrease of cost functional
$0^{\circ}$ Fix constants $s, \beta, \sigma$ such that $s>0, \beta \in(0,1)$ and $\sigma \in\left(0, \frac{1}{2}\right)$.
$1^{o}$ Try consequtively $k=\{0,1,2, \ldots\}$ and set $t=t^{k}=\beta^{m_{k}}$, where $m_{k}$ is the first non-negative integer $m$, for which the so-called Wolfe-condition is satisfied:

$$
\mathcal{J}\left(\mathbf{u}^{k}\right)-\mathcal{J}\left(\mathbf{u}^{k}+\beta^{m} s \mathbf{d}^{k}\right) \geq-\sigma \beta^{m} s \nabla \mathcal{J}\left(\mathbf{u}^{k}\right)^{T} \mathbf{d}^{k}
$$

Choice of free parameters, e.g., as $s=1.0, \beta=0.4$ and $\sigma=0.25$.

## Basic approaches (cont.):

- Quadratic interpolation: Approximate function $j$ using second-order polynomial $j(t) \simeq p(t)=a t^{2}+b t+c$. Setting $p^{\prime}(t)=2 a t+b=0$ yields to stepsize $t^{*}=-b /(2 a)$ when $a \neq 0$.
For determining the coefficients $a, b$ and $c$ usually two basic methods are applied.

1. first approach is based on using values of $j$ at three points, e.g.

$$
\begin{cases}t_{0}=0: & j_{0}=\mathcal{J}\left(\mathbf{u}^{k}\right) \\ t_{1}=\frac{1}{2}: & j_{1}=\mathcal{J}\left(\mathbf{u}^{k}+\frac{1}{2} \cdot \mathbf{d}^{k}\right) \\ t_{2}=1: & j_{2}=\mathcal{J}\left(\mathbf{u}^{k}+1 \cdot \mathbf{d}^{k}\right)\end{cases}
$$

Second-order polynomial that goes through the points $\left(t_{i}, j_{i}\right), i=1,2,3$, is recovered by solving the resulting linear problem, whose solution

$$
\left\{\begin{array}{l}
c=j_{0} \\
a=2\left(j_{0}-2 j_{1}+j_{2}\right) \\
b=-3 j_{0}+4 j_{1}-j_{2}
\end{array}\right.
$$

yields $t^{*}=\frac{-b}{2 a}=\frac{3 j_{0}-4 j_{1}+j_{2}}{4\left(j_{0}-2 j_{1}+j_{2}\right)}$.
2. if gradient of $\mathcal{J}$ is also available, then by using $j^{\prime}\left(t_{0}\right)=\nabla \mathcal{J}\left(\mathbf{u}^{k}\right)^{T} \mathbf{d}^{k}$ (cf. Definition 7), choosing $0<t_{1} \leq 1$ and setting $j_{1}=\mathcal{J}\left(\mathbf{u}^{k}+t_{1} \mathbf{d}^{k}\right)$, we get

$$
\left\{\begin{aligned}
c & =j_{0} \\
b & =\mathcal{J}\left(\mathbf{u}^{k}\right)^{T} \mathbf{d}^{k} \\
a & =\frac{j_{1}-b t_{1}-c}{t_{1}^{2}}
\end{aligned}\right.
$$

Notice that if $a<0$ then quadratic approximation is insufficient (too large search interval, bad search direction, etc.). Usually one then tries to decrease $I \longleftarrow 0.5 * I$ and repeat the process.

- Cubic interpolation: like the quadratic, but based on third-order polynomial approximation, which can be determined using four values of $j$ or two set of value-derivative pairs. Notice the more restrictive conditions for appropriate values of coefficients.
- more advanced example routine in lecture notes, see also MatLab Optimization Toolbox


## Descent direction:




## Descent direction (cont.):

- Starting point: from Theorem 7 it follows that

$$
-\nabla \mathcal{J}\left(\mathbf{u}^{k}\right)^{T} \nabla \mathcal{J}\left(\mathbf{u}^{k}\right)=-\left\|\nabla \mathcal{J}\left(\mathbf{u}^{k}\right)\right\|^{2}<0
$$

- in fact, $-\nabla \mathcal{J}\left(\mathbf{u}^{k}\right)$ points to the direction of the most rapid decrease
$\Rightarrow$ good direction, but usually not the best length!
- Newton's method:

$$
\mathbf{H}\left(\mathbf{u}^{k}\right) \mathbf{d}^{k}=-\nabla \mathcal{J}\left(\mathbf{u}^{k}\right)=-\mathbf{g}^{k}
$$

- well-defined when $\mathbf{H}\left(\mathbf{u}^{k}\right)$ positive definite (i.e., $\mathcal{J}$ strictly convex):

$$
\nabla \mathcal{J}\left(\mathbf{u}^{k}\right)^{T} \mathbf{d}^{k}=-\mathbf{g}^{k^{T}}\left[\mathbf{H}\left(\mathbf{u}^{k}\right)\right]^{-1} \mathbf{g}^{k}<0
$$

- BUT: analytic determination of $\mathbf{H}\left(\mathbf{u}^{k}\right)$ for real problems problematic!
- BUT: Inversion of $\mathbf{H}\left(\mathbf{u}^{k}\right)$ for real problems expensive!
- BFGS quasi-Newton method: approximate $\left(\mathbf{H}\left(\mathbf{u}^{k+1}\right)\right)^{-1}$ by

$$
\mathbf{D}^{k+1}=\mathbf{D}^{k}+\left(1+\frac{\mathbf{q}^{T} \mathbf{D}^{k} \mathbf{q}}{\mathbf{p}^{T} \mathbf{q}}\right) \frac{\mathbf{p} \mathbf{p}^{T}}{\mathbf{p}^{T} \mathbf{q}}-\frac{\mathbf{D}^{k} \mathbf{q} \mathbf{p}^{T}+\mathbf{p}\left(\mathbf{D}^{k} \mathbf{q}\right)^{T}}{\mathbf{p}^{T} \mathbf{q}}
$$

where

$$
\begin{aligned}
\mathbf{p} & =\mathbf{u}^{k+1}-\mathbf{u}^{k}, \\
\mathbf{q} & =\mathbf{g}^{k+1}-\mathbf{g}^{k}
\end{aligned}
$$

and usually $\mathbf{D}^{0}=\mathbf{D}^{1}=\mathbf{I}$.

- due to cumulation of errors reinitialization of $\mathbf{D}^{k}=\mathbf{I}$ after suitable number of iterations (usually after 20-50 iters.)


## Some additional stuff:

- Finite difference approximation of the gradient:
$\mathbf{g}_{i}^{k} \simeq \frac{\mathcal{J}\left(\mathbf{u}^{k}+h \delta_{i}\right)-\mathcal{J}\left(\mathbf{u}^{k}\right)}{h} \quad$ forward difference, 1st order accuracy wrt $h$, $\mathbf{g}_{i}^{k} \simeq \frac{\mathcal{J}\left(\mathbf{u}^{k}+h \delta_{i}\right)-\mathcal{J}\left(\mathbf{u}^{k}-h \delta_{i}\right)}{2 h} \quad$ central difference, 2nd order accuracy.
- the usual choice $h=\sqrt{\varepsilon}, \varepsilon$ is the machine epsilon (MATLAB eps).
- $\delta_{i}$ is the so-called Knonecker's delta

$$
\delta_{i}=\left\{\begin{array}{l}
1 i \text { th index } \\
0 \text { for other indeces }
\end{array}\right.
$$

- Levenberg-Marquart-method:
minimize $\quad \mathcal{J}(\mathbf{u})=\frac{1}{2} \sum_{i=1}^{N} \mathbf{e}_{i}(\mathbf{u})^{2}=\frac{1}{2} \mathbf{E}(\mathbf{u})^{T} \mathbf{E}(\mathbf{u}), \quad$ where $\mathbf{E}(\mathbf{u})=\left[\begin{array}{c}\mathbf{e}_{1}(\mathbf{u}) \\ \vdots \\ \mathbf{e}_{N}(\mathbf{u})\end{array}\right]$
- gradient: $\nabla \mathcal{J}(\mathbf{u})=\nabla\left(\frac{1}{2} \sum_{i} e_{i}(\mathbf{u})^{2}\right)=\sum_{i} \nabla e_{i}(\mathbf{u}) \cdot e_{i}(\mathbf{u})=\mathbf{J}(\mathbf{u})^{T} \mathbf{E}(\mathbf{u})$, where $\mathbf{J}(\mathbf{u})$ is the so-called Jacobian matrix

$$
\mathbf{J}(\mathbf{u})=\left[\begin{array}{ccc}
\frac{\partial \mathbf{e}_{1}(\mathbf{u})}{\partial \mathbf{u}_{1}} & \ldots & \frac{\partial \mathbf{e}_{1}(\mathbf{u})}{\partial \mathbf{u}_{n}} \\
\vdots & \ddots & \vdots \\
\frac{\partial \mathbf{e}_{N}(\mathbf{u})}{\partial \mathbf{u}_{1}} & \ldots & \frac{\partial \mathbf{e}_{N}(\mathbf{u})}{\partial \mathbf{u}_{n}}
\end{array}\right] \in \mathbf{R}^{N \times n} .
$$

- iteration: $\left(\mathbf{J}\left(\mathbf{u}^{k}\right)^{T} \mathbf{J}\left(\mathbf{u}^{k}\right)+\mu^{k} \mathbf{I}\right) \mathbf{d}^{k}=-\mathbf{J}\left(\mathbf{u}^{k}\right)^{T} \mathbf{E}\left(\mathbf{u}^{k}\right) \quad$ for suitable $\mu^{k}>0$.


## Some additional stuff (cont.):

## - Conjugate gradient method á la Polak-Ribière:

$$
\begin{aligned}
\mathbf{d}^{0} & =\mathbf{r}^{0}=-\nabla \mathcal{J}\left(\mathbf{u}^{0}\right) \quad \text { (initialization) } \\
t^{k} & : 1 \mathbf{D} \text { minimization of function } \mathcal{J}\left(\mathbf{u}^{k}+t^{k} \mathbf{d}^{k}\right) \\
\mathbf{u}^{k+1} & =\mathbf{u}^{k}+t^{k} \mathbf{d}^{k} \\
\mathbf{r}^{k+1} & =-\nabla \mathcal{J}\left(\mathbf{u}^{k+1}\right) \\
\beta^{k+1} & =\max \left\{\frac{\left(\mathbf{r}^{k+1}\right)^{T}\left(\mathbf{r}^{k+1}-\mathbf{r}^{k}\right)}{\left(\mathbf{r}^{k}\right)^{T} \mathbf{r}^{k}}, 0\right\} \\
\mathbf{d}^{k+1} & =\mathbf{r}^{k+1}+\beta^{k+1} \mathbf{d}^{k}
\end{aligned}
$$

- better control of search directions on (nearly) flat error surface
- de facto -method for solving SPD linear problems


## - About constrained optimization

- in many cases solution of an optimization problem should be constrained to a given admissible set $C$
- e.g., production costs always positive $u_{i} \geq 0 \quad \forall i$ (inequality constraint), eigenvector's norm always one $\left\|\mathbf{u}^{*}\right\|=1$ i.e. $\left\|\mathbf{u}^{*}\right\|-1=0$ (equality constraint) etc.
- most common approach is to complement the basic algorithm with a projection step:
4.5 Project $\mathbf{u}^{k+1}$ into $C$ by setting $\mathbf{u}^{k+1}=\mathcal{P}_{C}\left(\mathbf{u}^{k+1}\right)$.

Here $\mathcal{P}_{C}: \mathbf{R}^{n} \rightarrow \mathbf{R}^{n}$ is a projetion-operator, e.g.

$$
\begin{aligned}
\mathcal{P}_{\{\mathbf{u} \geq 0\}}(\mathbf{u}) & \equiv \max (\mathbf{u}, 0) \quad \text { (componentwise) } \\
\mathcal{P}_{\{\|\mathbf{u}\|=1\}}(\mathbf{u}) & \equiv \mathbf{u}=\frac{\mathbf{u}}{\|\mathbf{u}\|}
\end{aligned}
$$

- generally constraint optimization is a hard discipline
- Other basic approach is to use the so-called (augmented) Lagrangian (merit) function for combining cost function and constraints into one functional which is then minimized. This needs appropriate update rules for the resulting Lagrangian coefficients.

