## **Optimization in Machine Learning**

# Nonlinear programs Solvers



#### Learning goals

- Definition
- Max. Likelihood
- Normal regression
- Risk Minimization



#### SEQUENTIAL QUADRATIC PROGRAMMING

For simplification, we consider only equality constraints, thus problems of the form

$$\min f(\mathbf{x}) \qquad \text{s.t.} \quad h(\mathbf{x}) = 0.$$

#### Idea:

• Instead of *f* we optimize the 2nd order Taylor approximation in a point  $\tilde{x}$ 

$$\tilde{f}(\mathbf{x}) = f(\tilde{\mathbf{x}}) + \nabla_{x} f(\tilde{\mathbf{x}})^{T} (\mathbf{x} - \tilde{\mathbf{x}}) + \frac{1}{2} (\mathbf{x} - \tilde{\mathbf{x}})^{T} \nabla_{xx}^{2} f(\tilde{\mathbf{x}}) (\mathbf{x} - \tilde{\mathbf{x}})$$

• *h* is also replaced by its linear approximation in  $\tilde{x}$ .

$$\tilde{h}(\mathbf{x}) = h(\tilde{\mathbf{x}}) + \nabla h(\tilde{\mathbf{x}})^{\mathsf{T}}(\mathbf{x} - \tilde{\mathbf{x}}).$$



#### SEQUENTIAL QUADRATIC PROGRAMMING / 2

With  $d := (\mathbf{x} - \tilde{\mathbf{x}})$  we formulate the quadratic auxiliary problem

$$\min_{\boldsymbol{d}} \quad \tilde{f}(\boldsymbol{d}) := f(\tilde{\boldsymbol{x}}) + \boldsymbol{d}^T \nabla_x f(\tilde{\boldsymbol{x}}) + \frac{1}{2} \boldsymbol{d}^T \nabla_{xx}^2 f(\tilde{\boldsymbol{x}}) \boldsymbol{d}$$
s.t. 
$$\tilde{h}(\boldsymbol{d}) := h(\tilde{\boldsymbol{x}}) + \nabla h(\tilde{\boldsymbol{x}})^T \boldsymbol{d} = 0.$$

Even if no conditions for optimality can be formulated for the actual optimization problem, the KKT conditions apply in an optimum of this problem necessarily.

If the matrix  $\nabla_{xx}^2 f(\mathbf{x})$  is positive semidefinite, it is a **convex** optimization problem.

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#### **SEQUENTIAL QUADRATIC PROGRAMMING / 3**

Using the Lagrange function

$$L(\boldsymbol{d},\boldsymbol{\beta}) = \boldsymbol{d}^T \nabla_x f(\tilde{\boldsymbol{x}}) + \frac{1}{2} \boldsymbol{d}^T \nabla_{xx}^2 f(\tilde{\boldsymbol{x}}) \boldsymbol{d} + \boldsymbol{\beta}^T (h(\tilde{\boldsymbol{x}}) + \nabla h(\tilde{\boldsymbol{x}})^T \boldsymbol{d})$$

we formulate the KKT conditions

- $\nabla_{\boldsymbol{d}} L(\boldsymbol{d}, \boldsymbol{\beta}) = \nabla_{\boldsymbol{x}} f(\tilde{\boldsymbol{x}}) + \nabla_{\boldsymbol{x}\boldsymbol{x}}^2 f(\tilde{\boldsymbol{x}}) \boldsymbol{d} + \nabla h(\tilde{\boldsymbol{x}})^T \boldsymbol{\beta} = 0$
- $h(\tilde{\boldsymbol{x}}) + \nabla h(\tilde{\boldsymbol{x}})^T \boldsymbol{d} = 0$

or in matrix notation

$$\begin{pmatrix} \nabla_{xx}^2 f(\tilde{\boldsymbol{x}}) & \nabla h(\tilde{\boldsymbol{x}})^T \\ \nabla h(\tilde{\boldsymbol{x}}) & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{d} \\ \boldsymbol{\beta} \end{pmatrix} = - \begin{pmatrix} \nabla_x f(\tilde{\boldsymbol{x}}) \\ h(\tilde{\boldsymbol{x}}) \end{pmatrix}$$

The solution of the **quadratic subproblem** can thus be traced back to the solution of a linear system of equations.



### **SEQUENTIAL QUADRATIC PROGRAMMING / 4**

Algorithm SQP for problems with equality constraints

- 1: Select a feasible starting point  $\mathbf{x}^{(0)} \in \mathbb{R}^n$
- 2: while Stop criterion not fulfilled do
- 3: Solve quadratic subproblem by solving the equation

$$\begin{pmatrix} \nabla_{xx}^2 L(\mathbf{x}, \boldsymbol{\mu}) & \nabla h(\mathbf{x})^T \\ \nabla h(\mathbf{x}) & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{d} \\ \boldsymbol{\beta} \end{pmatrix} = - \begin{pmatrix} \nabla_x L(\mathbf{x}, \boldsymbol{\mu}) \\ h(\mathbf{x}) \end{pmatrix}$$

4: Set 
$$\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} + \mathbf{d}$$

5: end while

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#### PENALTY METHODS

**Idea:** Replace the constrained Optimization problem with a sequence of unconstrained optimization problems using a **penalty function**.

Instead of looking at

$$\min f(\mathbf{x}) \qquad \text{s.t.} \quad h(\mathbf{x}) = 0.$$

we look at the unconstrained optimization problem

$$\min_{\mathbf{x}} p(\mathbf{x}) = f(\mathbf{x}) + \rho \frac{\|h(\mathbf{x})\|^2}{2}.$$

Under appropriate conditions it can be shown that the solutions of the problem for  $\rho \to \infty$  converge against the solution of the initial problem.

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#### **BARRIER METHOD**

**Idea:** Establish a "barrier" that penalizes if **x** comes too close to the edge of the allowed set **S**. For the problem

$$\min f(\mathbf{x}) \qquad \text{s.t.} \quad g(\mathbf{x}) \leq 0$$

a common Barrier function is

$$\mathcal{B}_{
ho} = f(\mathbf{x}) - 
ho \sum_{i=1}^m \ln(-g_i(\mathbf{x}))$$

The penalty term becomes larger, the closer **x** comes to 0, i.e. the limit of the feasible set. Under certain conditions, the solutions of min  $B_{\rho}$  for  $\rho \rightarrow 0$  converge against the optimum of the original problem.

The procedure is also called interior-point method.

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## **Constrained Optimization in R**

### **CONSTRAINED OPTIMIZATION IN R**

- The function **optim(..., method = "L-BFGS-B")** uses quasi-newton methods and can handle box constraints.
- The function **nlminb()** uses trust-region procedures and can also handle box constraints.
- constrOptim() can be used for optimization problems with linear inequality conditions and is based on interior-point methods.
- **nloptr** is an interface to **NLopt**, an open-source library for nonlinear optimization

(https://nlopt.readthedocs.io/en/latest/)

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