Optimization in Machine Learning

Nonlinear programs Solvers

Learning goals

- **O** 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 *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 $\tilde{\textbf{x}}$.

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

SEQUENTIAL QUADRATIC PROGRAMMING / 2

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

$$
\min_{\mathbf{d}} \qquad \tilde{f}(\mathbf{d}) := f(\tilde{\mathbf{x}}) + \mathbf{d}^T \nabla_{\mathbf{x}} f(\tilde{\mathbf{x}}) + \frac{1}{2} \mathbf{d}^T \nabla_{\mathbf{x}\mathbf{x}}^2 f(\tilde{\mathbf{x}}) \mathbf{d}
$$
\ns.t.
$$
\tilde{h}(\mathbf{d}) := h(\tilde{\mathbf{x}}) + \nabla h(\tilde{\mathbf{x}})^T \mathbf{d} = 0.
$$

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 ∇² *xx f*(**x**) is positive semidefinite, it is a **convex optimization problem**.

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SEQUENTIAL QUADRATIC PROGRAMMING / 3

Using the Lagrange function

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

we formulate the KKT conditions

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

or in matrix notation

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

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

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

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

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

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. \times \times

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 $f(\mathbf{x})$ s.t. $g(\mathbf{x}) \leq 0$

a common **Barrier function** is

$$
B_{\rho} = f(\mathbf{x}) - \rho \sum_{i=1}^{m} \ln(-g_i(\mathbf{x}))
$$

 $\overline{\mathbf{X}}$

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_{ρ} for $\rho \rightarrow 0$ converge against the optimum of the original problem.

The procedure is also called **interior-point method**.

\mathbf{y} \overline{x}

[Constrained Optimization in R](#page-7-0)

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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