Today:
- constrained opt.
- interpolation

Announcements:
- Examlet 3
Levenberg-Marquardt

\[ \| \mathbf{\delta} (\hat{x}) \|_2 \]

If Gauss-Newton on its own is poorly, conditioned, can try Levenberg-Marquardt:

\[
\mathbb{J}_r \mathbb{J}_r (x_n) \mathbf{\delta}_n = \mathbb{J}_r (x_n) \mathbf{v} (x_n) \\
\mathbb{J}(x_n) \hat{\mathbf{\delta}}_n \equiv -\mathbf{v} (x_n)
\]

\[
\mathbb{J}_r \mathbb{J}_r (x_n) \mathbf{\delta}_n + \mu \mathbb{I} \mathbf{\delta}_n - \mathbb{J}_r (x_n) \mathbf{v} (x_n) \\
\mathbb{J}(x_n) \mathbf{\delta}_n \equiv \begin{bmatrix} -\mathbf{v} (x_n) \\ \mathbf{0} \end{bmatrix}
\]

\[
\left[ \begin{bmatrix} \mathbb{J}_n (x_n) \\ \sqrt{\mu} \mathbb{I} \end{bmatrix} \right] \hat{\mathbf{\delta}}_n \equiv \begin{bmatrix} -\mathbf{v} (x_n) \\ \mathbf{0} \end{bmatrix}
\]
Constrained Optimization: Problem Setup

Want $x^*$ so that

$$f(x^*) = \min_x f(x) \quad \text{subject to} \quad g(x) = 0$$

No inequality constraints just yet. This is equality-constrained optimization. Develop a necessary condition for a minimum.

Unconstrained: $\nabla f(x^*) = 0$

$s$ is a feasible direction if I can find an $r$ so that for all $(q,r)$:

$$g(x + \alpha s) = 0$$
Constrained Optimization: Necessary Condition

\[ \text{constr. } \min_{x} f(x) \Rightarrow \nabla f(x^*) \cdot \hat{s} \geq 0 \]  

"uphill in all feasible directions"

On the interior of \( \{ g(i) = 0 \} \), \( \hat{s} \) and \( -\hat{s} \) are feasible; 

\[ \nabla f(x^*) \cdot \hat{s} \geq 0 \quad \text{and} \quad \nabla f(x^*) \cdot (-\hat{s}) \geq 0 \]

\[ \Rightarrow \nabla f(x) = 0 \]
- \Delta f + \text{level set of } g \text{ through } x^* \\
\therefore - \Delta f = \chi \wedge Dg
\[ g : \mathbb{R}^n \rightarrow \mathbb{R} \]

\[ \nabla f = \nabla g \]

\[ \mathcal{J}_g : \mathbb{R}^n \rightarrow \mathbb{R}^n \]

\[ \nabla f = \bigcup_{\partial g}^\lambda \left( \frac{\partial}{\partial g} \right) \]

\[ \nabla f \in \text{row span } (\mathcal{J}_g) \]

\( \uparrow \) necessary cond.
Lagrange Multipliers

Seen: Need $-\nabla f(x) = J^T_g \lambda$ at the (constrained) optimum.

Idea: Turn constrained optimization problem for $x$ into an *unconstrained* optimization problem for $(x, \lambda)$. How?

$$L(x, \lambda) = f(x) + \lambda^T g(x)$$

Idea: run unconstrained opt.
Lagrangian Multipliers: Development

\[ \mathcal{L}(x, \lambda) := f(x) + \lambda^T g(x). \]

\[ 0 = \nabla \mathcal{L} = \begin{bmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial x} + \frac{\partial g}{\partial x} \lambda \end{bmatrix} = \begin{bmatrix} \nabla f(x) \\ \nabla g(x) \lambda \end{bmatrix} \]

For example: use Newton to minimize \( \mathcal{L} \)

"SQP": Sequential Quadratic Programming

**Demo:** Sequential Quadratic Programming
Inequality-Constrained Optimization

Want $x^*$ so that

$$f(x^*) = \min_x f(x) \quad \text{subject to} \quad g(x) = 0 \quad \text{and} \quad h(x) \leq 0$$

This is *inequality-constrained optimization*. Develop a necessary condition for a minimum.

$$\nabla y = 0 \Rightarrow h(x) \leq 0 \quad \bar{g}(x) = \begin{cases} 1 & h(x) > 0 \\ 0 & h(x) \leq 0 \end{cases}$$

$$L(x, \lambda_1, \lambda_2) = f(x) + \lambda_1^T g(x) + \lambda_2^T h(x)$$

Ineq. constraints can be active or inactive.

If constraint is active: $h_i(x) = 0$
If $h_i$ is inactive, must $(\lambda_i)_i = 0$.

If $h_i$ is active: Behavior of $h_i$ could change the minimum $h_i(x) = 0$.

$(\forall \lambda): \cdot h_i = 0$ implies $h_i$ is active exactly on the boundary.

Complementarity condition
Inequality-Constrained Optimization (cont’d)

Develop a set of necessary conditions for a minimum.

\[
\nabla_x \mathcal{L}(\mathbf{x}, \mathbf{y}, \mathbf{\lambda}) = 0 \\
g(\mathbf{x}) = 0 \\
\rightarrow \mathbf{h}(\mathbf{x})^T \mathbf{\lambda} = 0 \\
\mathbf{h}(\mathbf{x}) \leq 0 \\
\Rightarrow \mathbf{\lambda} \geq 0 \quad \text{c- sign convention on } \mathbf{\lambda}_i
\]
Outline

Introduction to Scientific Computing

Systems of Linear Equations

Linear Least Squares

Eigenvalue Problems

Nonlinear Equations

Optimization

Interpolation
  Introduction and Methods

Numerical Integration and Differentiation

Initial Value Problems for ODEs

Boundary Value Problems for ODEs

Partial Differential Equations and Sparse Linear Algebra

Fast Fourier Transform

Additional Topics