

Today:

- constrained opt.
- interpolation

Announcements:

- Example 3

Levenberg-Marquardt

$$\|r(x)\|_2$$

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

$$J^T J(x_k) \vec{s}_k = -J^T(x_k) v(x_k)$$

$$\Leftrightarrow J(x_k) \vec{s}_k \approx -v(x_k)$$

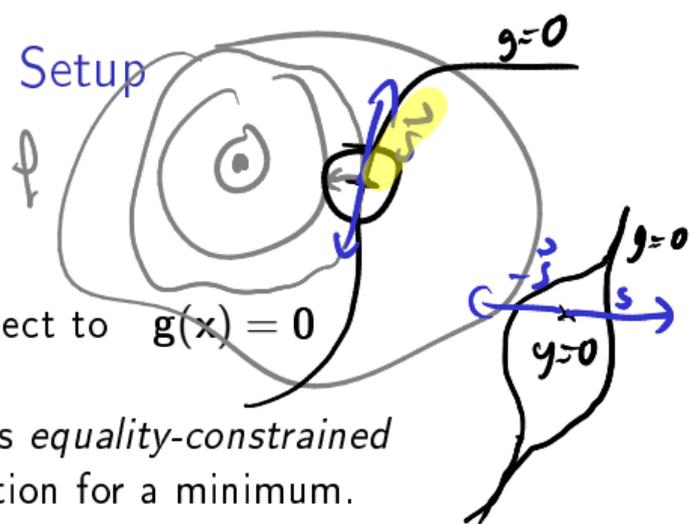
$$J^T J(x_k) \vec{s}_k + \mu_k I_n \vec{s}_k = -J^T(x_k) v(x_k)$$

$$\Leftrightarrow \begin{bmatrix} J^T J(x_k) \\ \sqrt{\mu_k} \end{bmatrix} \vec{s}_k \approx \begin{bmatrix} -v(x_k) \\ 0 \end{bmatrix}$$

Constrained Optimization: Problem Setup

Want x^* so that

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

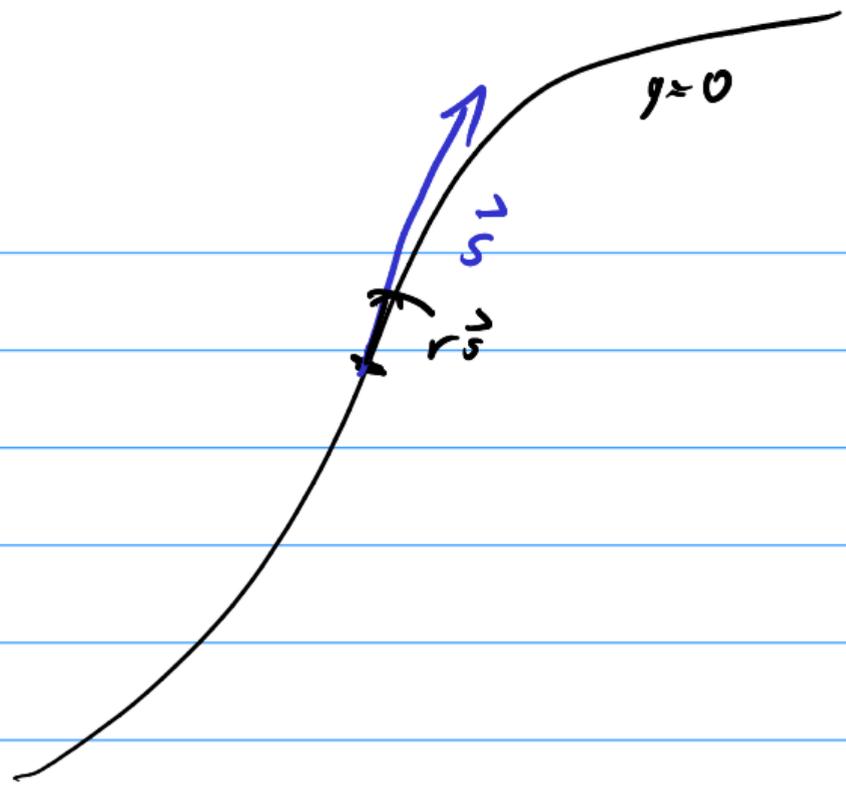


No inequality constraints just yet. This is *equality-constrained optimization*. Develop a necessary condition for a minimum.

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

At x w/ $g(x) \neq 0$, \vec{s} is a feasible direction if I can find a α, r

so that for $\alpha \in (0, r)$: $y\left(\begin{matrix} \vec{s} \\ x + \alpha \vec{s} \end{matrix}\right) = 0$



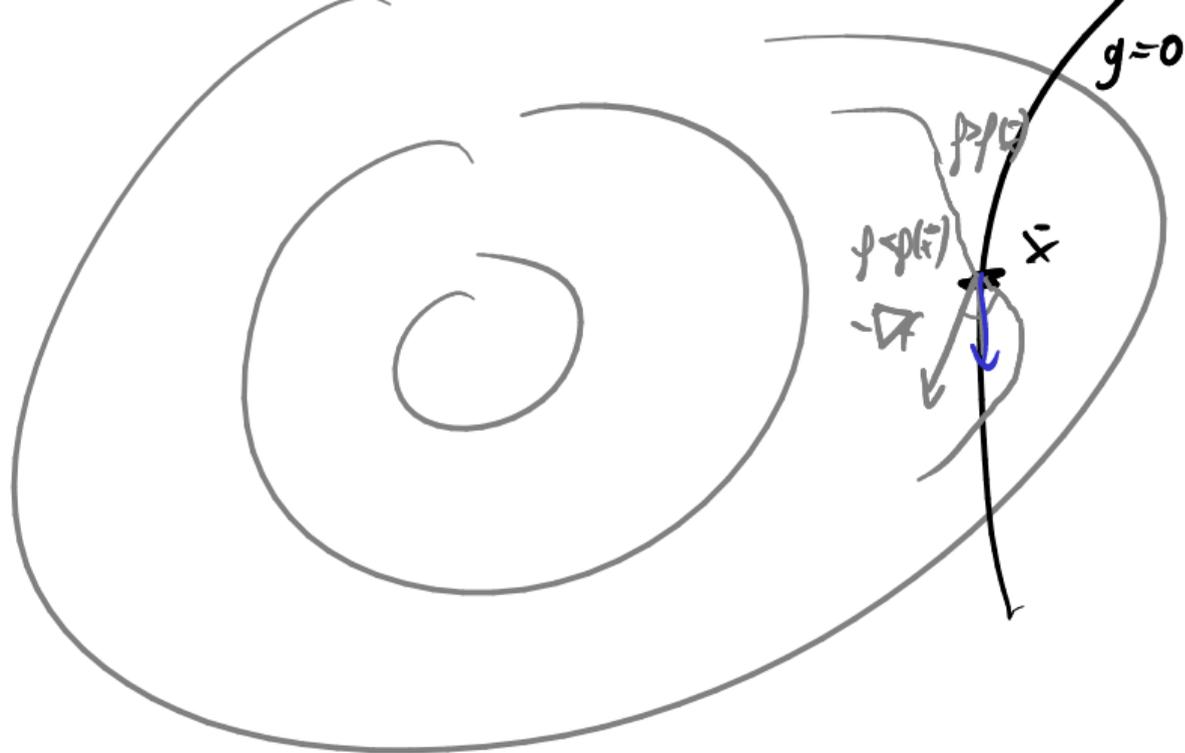
Constrained Optimization: Necessary Condition

constr. min at x^* \Rightarrow

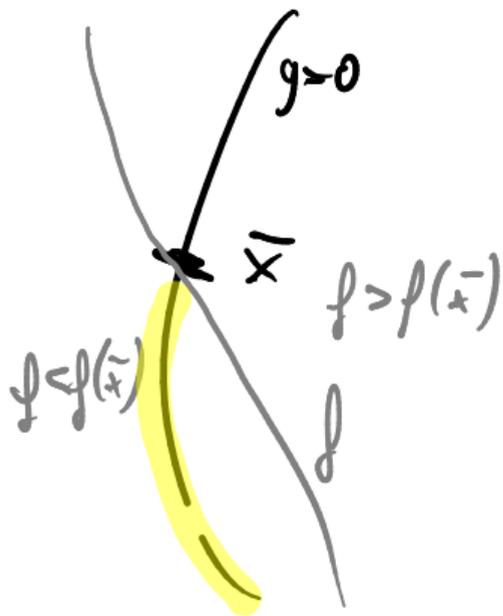
$$\nabla f(x^*) \cdot \vec{s} \geq 0 \quad \text{"uphill in all feasible directions"}$$

On the interior of $\{g(x) = 0\}$, \vec{s} and $-\vec{s}$ are feasible;

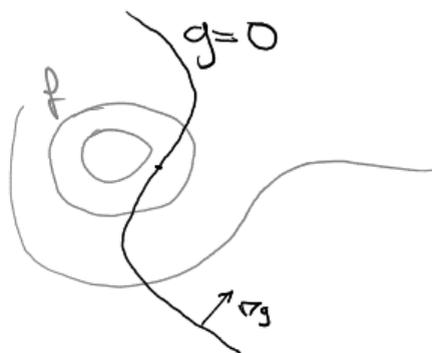
$$\nabla f(x^*) \cdot \vec{s} \geq 0 \quad \text{and} \quad \nabla f(x^*) \cdot (-\vec{s}) \geq 0$$
$$\Rightarrow \nabla f(x^*) = 0$$



$-\nabla f \perp$ level set of g through x^*
 $\Leftrightarrow -\nabla f = \lambda \nabla g$



Lagrange Multipliers



Seen: Need $-\nabla f(\mathbf{x}) = J_{\mathbf{g}}^T \lambda$ at the (constrained) optimum.

Idea: Turn constrained optimization problem for \mathbf{x} into an *unconstrained* optimization problem for (\mathbf{x}, λ) . How?

$$\mathcal{L}(\vec{x}, \vec{\lambda}) = f(\vec{x}) + \lambda^T g(\vec{x})$$

↑
Idea: run unconstrained opt.

Lagrange Multipliers: Development

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

$$0 = \nabla \mathcal{L} = \begin{bmatrix} \nabla_x \mathcal{L} \\ \nabla_\lambda \mathcal{L} \end{bmatrix} = \begin{bmatrix} \nabla f + \sum_j \lambda_j \nabla g_j(x) \\ g(x) \end{bmatrix}$$

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.

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

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

ineq. constraints can be active or inactive
if active $\forall h_i(x) = 0$

$\rightarrow h_i < 0$
If h_i is inactive: must $(\lambda_2)_i = 0$

If h_i is active: Behavior of h_i

$h_i = 0$ could change the minimum
 $h_i(x) = 0$

$$(\lambda_2)_i \cdot h_i = 0$$



complementarity condition

\Rightarrow turns h_i "on" / "active" exactly on the bdr.

Inequality-Constrained Optimization (cont'd)

Develop a set of necessary conditions for a minimum.

$$\nabla_x \mathcal{L}(x^*, \lambda_1^*, \lambda_2^*) = 0$$

$$g(x^*) = 0$$

$$\rightarrow h^T(x^*) \cdot \lambda_2 = 0$$

$$h(x^*) \leq 0$$

$$\rightarrow \lambda_2 \geq 0 \quad \leftarrow \text{sign convention only}$$

← feeds
Newton

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