Control and detection of immersed objects
Part III - Numerical methods

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Outline

The problem

Suppose we want to fit a function of the form

$$g(x) = \sum_{i=1}^{m} \alpha_i \phi_i(x)$$

to the data $\{(x_k, g_k),\ k = 1 : n\}$, where $n > m$. These data may correspond, for instance, to measured quantities g_k at the observation points x_k. The basis functions $\phi_1, \ldots, \phi_m$ are given and the function g is determined by the parameters $\alpha_1, \ldots, \alpha_m$.
By the least squares criterion we have to minimize

$$Q(\alpha) := \sum_{k=1}^{n} [g_k - g(x_k)]^2 = \sum_{k=1}^{n} \left[g_k - \sum_{i=1}^{m} \alpha_i \phi_i(x_k) \right]^2 = \sum_{k=1}^{n} R_k(\alpha)^2$$

The least squares method was first described by Carl Friedrich Gauss around 1794.

The problem

The least squares criterion consists in minimizing

$$Q(\alpha) = R(\alpha) \cdot R(\alpha)$$

with $R : \mathbb{R}^m \longrightarrow \mathbb{R}^n$ defined by

$$R_k(\alpha) = g_k - \sum_{i=1}^{m} \alpha_i \phi_i(x_k) \quad (k = 1 : n).$$

The Jacobian matrix of R is independent of α and given by

$$J_R = -\begin{bmatrix} \phi_1(x_1) & \dots & \phi_m(x_1) \\ \dots & \dots & \dots \\ \phi_1(x_n) & \dots & \phi_m(x_n) \end{bmatrix} \in \mathbb{R}^{n\times m}$$

Linear least squares method

Let $R : \mathbb{R}^m \rightarrow \mathbb{R}^n$ be a linear function of the parameters $\alpha_1, ..., \alpha_m$ and consider the least squares problem of finding

$$\arg\,\min_{\alpha \in \mathbb{R}^m} Q(\alpha)$$

where $Q(\alpha) := \sum_{i=1}^{n} (R_i(\alpha))^2 = R(\alpha) \cdot R(\alpha)$.

Since R is a linear function of α, we have

$$R(\alpha) = R(0) + J_R \alpha$$

where the Jacobian matrix $J_R \in \mathbb{R}^{n \times m}$ is independent of α. Then

$$\begin{aligned} Q(\alpha) &= R(\alpha) \cdot R(\alpha) = R(\alpha)^T R(\alpha) \\ &= R(0) \cdot R(0) + 2\alpha^T J_R^T R(0) + \alpha^T J_R^T J_R \alpha \end{aligned}$$

More specifically

Recall the Jacobian matrix of R

$$J_R = \begin{bmatrix} \phi_1(x_1) & \dots & \phi_m(x_1) \\ \dots & \dots & \dots \\ \phi_1(x_n) & \dots & \phi_m(x_n) \end{bmatrix} \in \mathbb{R}^{m \times n}$$

Then

$$J_R^T J_R = \begin{bmatrix} (\phi_1, \phi_1) & \dots & (\phi_1, \phi_m) \\ \vdots & \vdots & \vdots \\ (\phi_m, \phi_1) & \dots & (\phi_m, \phi_m) \end{bmatrix} \in \mathbb{R}^{m \times m}$$

with

$$(\phi_i, \phi_j) := \sum_{k=1}^{n} \phi_i(x_k)\phi_j(x_k)$$

Linear least squares method

Recall that

$$Q(\alpha) = R(0) \cdot R(0) + 2\alpha^T J_R^T R(0) + \alpha^T J_R^T J_R \alpha$$

ie, Q is a quadratic function of the parameters $\alpha_1, ..., \alpha_m$.
A unique minimizer of Q exists provided the linear system

$$\nabla Q(\alpha) = 0 \Leftrightarrow J_R^T J_R \alpha = -J_R^T R(0)$$

has a unique solution α^* and $D^2 Q(\alpha^*) = J_R^T J_R$ is positive definite.

If the columns of J_R are linearly independent then $J_R^T J_R$ is positive definite and Q has a unique minimizer α^* which can be found by solving the normal system.

Observe that the matrix $J_R^T J_R \in \mathbb{R}^{m \times m}$ is certainly positive semidefinite.

More specifically

Recall that

$$R_k(\alpha) = g_k - \sum_{i=1}^{m} \alpha_i \phi_i(x_k) \quad (k = 1 : n).$$

Let $g = [g_1, ..., g_n]^T$. Then

$$R(0) = g$$

and

$$-J_R^T R(0) = \begin{bmatrix} (\phi_1, g) \\ \vdots \\ (\phi_m, g) \end{bmatrix} \in \mathbb{R}^m$$

with

$$(\phi_i, g) := \sum_{k=1}^{n} \phi_i(x_k) g_k$$

More specifically

Hence, when

$$R_k(\alpha) = g_k - \sum_{i=1}^{m} \alpha_i \phi_i(x_k) \quad (k = 1 : n),$$

the linear system

$$J_R^T J_R \alpha = -J_R^T R(0)$$

is the normal system

$$\begin{bmatrix} (\phi_1, \phi_1) & \dots & (\phi_1, \phi_n) \\ \vdots & \vdots & \vdots \\ (\phi_n, \phi_1) & \dots & (\phi_n, \phi_n) \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{bmatrix} = \begin{bmatrix} (\phi_1, g) \\ \vdots \\ (\phi_n, g) \end{bmatrix}$$

The matrix of this system is positive definite if and only if the basis functions $\phi_1, ..., \phi_m$ are linearly independent on the set $\{x_1, ..., x_n\}$.

The 2-D Stokes fundamental solution

Fundamental solution (U, P) of the two-dimensional Stokes equations

$$U(x) = -\frac{1}{4\pi}\left(-I\log(|x|) + \frac{x \otimes x}{|x|^2}\right),$$
$$P(x) = -\frac{1}{2\pi}\frac{x}{|x|^2}.$$

More precisely

$$U_{ij}(x) = -\frac{1}{4\pi}\left(-\delta_{ij}\log(|x|) + \frac{x_i x_j}{|x|^2}\right),$$
$$P_i(x) = -\frac{1}{2\pi}\frac{x_i}{|x|^2} \quad (i, j = 1, 2).$$

Note that U and P have a singularity at the origin.

The 2-D Stokes fundamental solution

Recall that the Dirac delta δ_b $(b \in \Omega)$ is a linear functional on the space of test functions $C^\infty(\overline{\Omega})$, defined by

$$\delta_b[\varphi] = \varphi(b),$$

for every test function φ. A convenient abuse of notation is

$$\int_\Omega \delta_b(x)\varphi(x)dx = \varphi(b),\ \varphi \in C^\infty(\overline{\Omega}).$$

For each $j = 1, 2$, the pair (U_j, P_j) given by

$$U_j(x) := U(x)e_j = -\frac{1}{4\pi}\left(-\log\left(|x|\right)e_j + \frac{x_j x}{|x|^2}\right),$$
$$P_j(x) := P(x)e_j = -\frac{1}{2\pi}\frac{x_j}{|x|^2} \quad (j = 1, 2)$$

satisfies

$$\left.\begin{array}{l} \Delta U_j - \nabla P_j = \delta_0 e_j \\ \nabla \cdot U_j = 0 \end{array}\right\} \text{ in } \mathbb{R}^2$$

The 2-D Stokes fundamental solution

Remark $\delta_0 e_j$ represents a concentrated point force in the e_j direction, located at the origin

From

$$\left.\begin{array}{l}\Delta U_j - \nabla P_j = \delta_0 e_j \\ \nabla \cdot U_j = 0\end{array}\right\} \text{ in } \mathbb{R}^2$$

it follows that

$$\begin{array}{l}\Delta U_j(x) - \nabla P_j(x) = 0 \text{ for } x \neq 0 \\ \nabla \cdot U_j(x) = 0 \text{ for } x \neq 0\end{array}$$

and

$$\begin{array}{l}\Delta U_j(x-y) - \nabla P_j(x-y) = 0 \text{ for } x \neq y \\ \nabla \cdot U_j(x-y) = 0 \text{ for } x \neq y\end{array}$$

Note that, for each $y \in \mathbb{R}^2$, the functions u and p defined by

$$(u(x), p(x)) = (U_j(x-y), P_j(x-y)) \quad (j = 1, 2)$$

have a singularity at $x = y$.

Numerical solution for the Stokes equations

Consider the Stokes system

$$\begin{aligned} \Delta u - \nabla p &= 0 \text{ in } \Omega \\ \nabla \cdot u &= 0 \text{ in } \Omega \\ u &= u_* \text{ on } \Sigma := \partial\Omega \end{aligned}$$

where Ω and u_* are known. Our aim is to solve numerically this problem, ie, to construct an approximating solution $(\tilde{u}, \tilde{p})$.

Observe that for every $y \notin \overline{\Omega}$ the pair (u, p) defined by

$$(u(x), p(x)) = (U_j(x - y), P_j(x - y)) \quad (j = 1, 2)$$

satisfy

$$\begin{aligned} \Delta u - \nabla p &= 0 \text{ in } \Omega \\ \nabla \cdot u &= 0 \text{ in } \Omega \end{aligned}$$

but the boundary condition $u = u_*$ is not satisfied.

The artificial boundary

The idea is to look for an approximation of (u, p) of the form

$$\tilde{u}(x) = \sum_{j=1}^{2} \sum_{y_i \notin \overline{\Omega}} a_{ji} U_j(x - y_i),$$

$$\tilde{p}(x) = \sum_{j=1}^{2} \sum_{y_i \notin \overline{\Omega}} a_{ji} P_j(x - y_i)$$

Let Ω, $\hat{\Omega}$ be connected bounded domains with regular boundaries

$$\Sigma := \partial\Omega \text{ and } \hat{\Omega} := \partial\hat{\Omega}.$$

If $\overline{\Omega} \subset \hat{\Omega}$, we say that the artificial boundary $\hat{\Sigma}$ is an admissible source set associated to Σ.

The Method of Fundamental Solutions (MFS)

We consider a finite number of points $y_1, ..., y_m$ in $\hat{\Sigma}$ and the associated basis functions defined by

$$U_j(x - y_i)|_\Sigma \text{ with } y_i \in \hat{\Sigma}, \quad i = 1 : m, \quad j = 1, 2.$$

The approximation of (u, p) is of the form

$$\tilde{u}(x) = \sum_{j=1}^{2} \sum_{i=1}^{m} a_{ji} U_j(x - y_i) = \sum_{i=1}^{m} U(x - y_i) a_i,$$

$$\tilde{p}(x) = \sum_{j=1}^{2} \sum_{i=1}^{m} a_{ji} P_j(x - y_i) = \sum_{i=1}^{m} P(x - y_i) \cdot a_i, \quad a_i = \begin{bmatrix} a_{1i} \\ a_{2i} \end{bmatrix}$$

Observe that

$$\Delta \tilde{u} - \nabla \tilde{p} = 0 \quad \nabla \cdot \tilde{u} = 0 \text{ in } \Omega.$$

The Method of Fundamental Solutions (MFS)

The coefficients a_{ji} can be calculated by linear least squares, in order to fit the boundary data $u_*(x_k)$ at a finite number of points x_k.

Take $x_1, ..., x_M \in \Sigma$, with $M > m$, and consider the minimization of

$$Q(a) = \sum_{k=1}^{M} \left| \sum_{j=1}^{2} \sum_{i=1}^{m} a_{ji} U_j(x_k - y_i) - u_*(x_k) \right|^2$$

This leads to the resolution of a linear system

$$\mathbb{M}^T \cdot \mathbb{M} \cdot a = \mathbb{M}^T \cdot \mathbb{G}$$

The Method of Fundamental Solutions (MFS)

In the linear system $\mathbb{M}^T \cdot \mathbb{M} \cdot a = \mathbb{M}^T \cdot \mathbb{G}$

$$\mathbb{M} = \begin{bmatrix} U(x_1 - y_1) & \dots & U(x_1 - y_m) \\ \vdots & \ddots & \vdots \\ U(x_M - y_1) & \dots & U(x_M - y_m) \end{bmatrix} \qquad a = \begin{bmatrix} a_1 \\ \vdots \\ a_m \end{bmatrix} = \begin{bmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{1m} \\ a_{2m} \end{bmatrix}$$

$$\mathbb{G} = \begin{bmatrix} u_*(x_1) \\ \vdots \\ u_*(x_M) \end{bmatrix} = \begin{bmatrix} (u_*)_1(x_1) \\ (u_*)_2(x_1) \\ \vdots \\ (u_*)_1(x_M) \\ (u_*)_2(x_M) \end{bmatrix}$$

Example

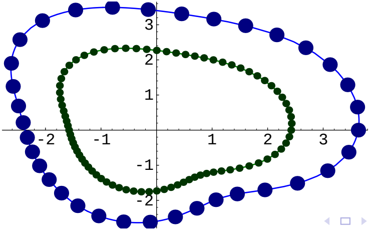
We consider the steady Stokes flow given by
$u(x_1, x_2) = 2x_1x_2e_1 - x_2^2e_2$ and $p(x_1, x_2) = -2x_2$ in the interior domain whose boundary is parametrized by

$$\Sigma(t) = r(t)(\cos(t)e_1 + \sin(t)e_2), \quad t \in [0, 2\pi],$$

with $r(t) = 2 + \sin(t + \cos(2t))/2$. The artificial boundary $\hat{\Gamma}$ is parametrized by

$$\hat{\Sigma}(t) = \hat{r}(t)(\cos(t)e_1 + \sin(t)e_2), \quad t \in [0, 2\pi], \quad \text{with } \hat{r} = 1.5r.$$

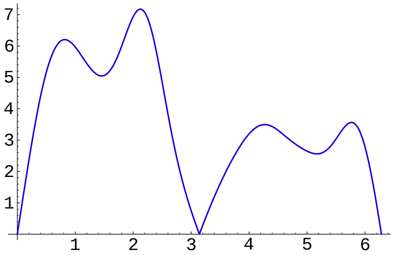
In the simulations we will take $M = 80$ points on Σ and $m = 35$ points forces on $\hat{\Sigma}$.

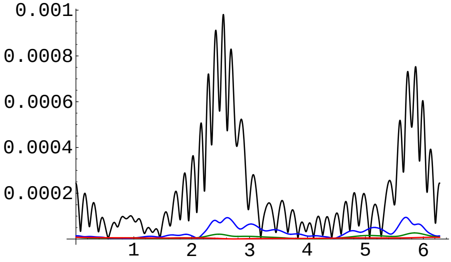


Example (contd.)

In the figures we show

- the plot of $|u|$ on the boundary, which is not visually distinct from the approximation given by the MFS
- the error plot, which presents relative errors smaller than 0.05% . On the right we also show other smaller lines, with the error plot in interior curves, showing that the error decreases significantly in the interior of Ω.





The Gauss-Newton Method

Let $R : \mathbb{R}^m \to \mathbb{R}^n$ and consider the nonlinear least squares problem of finding

$$\arg\min_{\alpha \in \mathbb{R}^m} F(\alpha)$$

where $F(\alpha) := \sum_{i=1}^{n} (R_i(\alpha))^2 = R(\alpha) \cdot R(\alpha)$ and R is a nonlinear function of α.

Suppose α_{prev} is an approximation for the minimizer and look for a better approximation $\alpha_{new} = \alpha_{prev} + h$.

For $\alpha \in \mathbb{R}^m$ and $h \in \mathbb{R}^m$ with $|h|$ small, we consider the linear approximation

$$R(\alpha + h) \simeq R(\alpha) + J_R(\alpha) h := \mathcal{L}(h).$$

Then

$$\begin{aligned} F(\alpha + h) &\simeq \mathcal{L}(h) \cdot \mathcal{L}(h) \\ &= R(\alpha) \cdot R(\alpha) + 2h^T J_R^T(\alpha) R(\alpha) + h^T J_R^T(\alpha) J_R(\alpha) h \end{aligned}$$

The Gauss-Newton Method

In order to determine h, the correction for α_{prev}, consider the approximation by a quadratic function

$$F(\alpha_{prev} + h) \simeq R(\alpha_{prev}) \cdot R(\alpha_{prev}) + 2h^T J_R^T(\alpha_{prev}) R(\alpha_{prev}) \\ + h^T J_R^T(\alpha_{prev}) J_R(\alpha_{prev}) h := \mathcal{Q}(h)$$

and the linear least squares problem of finding

$$h_{GN} = \arg\min_{h \in \mathbb{R}^m} \mathcal{Q}(h).$$

Now, the gradient and Hessian matrix of $\mathcal{Q}$ are given by

$$\nabla \mathcal{Q}(h) = 2 J_R^T(\alpha_{prev}) R(\alpha_{prev}) + 2 J_R^T(\alpha_{prev}) J_R(\alpha_{prev}) h$$

$$D^2 \mathcal{Q}(h) = 2 J_R^T(\alpha_{prev}) J_R(\alpha_{prev}) \text{ independent of } h$$

The Gauss-Newton Method

A unique minimizer of $\mathcal{Q}$ exists provided the normal system

$$J_R^T(\alpha_{prev})J_R(\alpha_{prev})h = -J_R^T(\alpha_{prev})R(\alpha_{prev}) \Leftrightarrow \nabla\mathcal{Q}(h) = 0$$

has a unique solution h_{GN} and $J_R^T(\alpha_{prev})J_R(\alpha_{prev}) = D^2\mathcal{Q}(h_{GN})$ is positive definite.

If the columns of $J_R(\alpha_{prev})$ are linearly independent then $J_R^T(\alpha_{prev})J_R(\alpha_{prev})$ is positive definite and $\mathcal{Q}$ has a unique minimizer h_{GN} which can be found by solving the above normal system.

Observe that the matrix $J_R^T(\alpha_{prev})J_R(\alpha_{prev})$ is certainly positive semidefinite.

The Levenberg-Marquardt Algorithm (LMA)

Levenberg (1944) and later Marquardt (1963) suggested to use a damped Gauss-Newton method. The correction h for finding a new approximation $\alpha_{new} = \alpha_{prev} + h_{LM}$ is obtained by defining the following modification of the normal system

$$[J_R^T(\alpha_{prev})J_R(\alpha_{prev}) + \lambda I]h_{LM} = -J_R^T(\alpha_{prev})R(\alpha_{prev}), \quad \lambda \geq 0.$$

Observe that the matrix $J_R^T(\alpha_{prev})J_R(\alpha_{prev}) + \lambda I$ is positive definite when $\lambda > 0$.

The appropriated value of λ is calculated during the iterative procedure.

The damping parameter in the LMA

$$[J_R^T(\alpha_{prev})J_R(\alpha_{prev}) + \lambda I]h_{LM} = -J_R^T(\alpha_{prev})R(\alpha_{prev}), \quad \lambda \geq 0.$$

- For large values of λ, we get

$$h_{LM} \simeq -\frac{J_R^T(\alpha_{prev})R(\alpha_{prev})}{\lambda} = -\frac{\nabla F(\alpha_{prev})}{2\lambda}$$

  i.e, a short step in the steepest descent direction. This is good if the current iterate is far from the solution.
- If λ is very small, then $h_{LM} \simeq h_{GN}$, which is a good step in the final stages of the iteration.