Exploring Local Solution Manifolds of Nonlinear Least Squares Problems

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Motivation

- Parameter estimation in some computational neuroscience models often results in non-unique solutions.
- Study when nontrivial solution sets exist in rank-deficient least squares problems.
- **Goal**: Identify solution manifold

Rank-Deficient Least Squares

- $R : \mathbb{R}^n \to \mathbb{R}^m$, $m > n$ with Jacobian $J : \mathbb{R}^n \to \mathbb{R}^{m\times n}$ of rank r, least squares problem is
$$\min_{p\in\mathbb{R}^n} f(p), \qquad f(p) = \frac{1}{2}\|R(p)\|_2^2 = \frac{1}{2}\sum_{i=1}^{m} R_i(p)^2$$
- Solution set:
$$\mathcal{M} = \left\{ p^* \in \mathbb{R}^n \;:\; \|R(p^*)\|_2^2 = \min_{p\in\mathbb{R}^n} \|R(p)\|_2^2 \right\}$$
- Necessary optimality conditions for $p^* \in \mathcal{M}$:
$$\nabla f(p^*) = 0 \quad \text{and} \quad \nabla^2 f(p^*) \succeq 0$$
- If $\nabla^2 f(p^*) \succ 0$, then p^* is a strict local minimizer. For a nontrivial solution set to exist locally, must have $\nabla^2 f(p^*) \not\succ 0$.

  Occurs when $R(p^*) = 0$ and $r < n$.
- **Linear case**: For $A \in \mathbb{R}^{m\times n}$ of rank r and $b \in \mathbb{R}^m$, solve
$$\min_{p\in\mathbb{R}^n} f(p), \qquad f(p) = \frac{1}{2}\|Ap - b\|_2^2$$
- Using SVD $A = U\Sigma V^T$, can parameterize linear solution set as
$$\mathcal{M} = \left\{ p^* + V_{n-r}\, q \;:\; q \in \mathbb{R}^{n-r} \right\}, \quad V = \left[V_r\; V_{n-r}\right]$$

Levenberg-Marquardt Algorithm

- Use Levenberg-Marquardt described in [3] to solve least squares.
- Given $J = J(x_k)$, $R = R(x_k)$, new iterate $x_{k+1} = x_k + s$ where
$$\left(J^T J + \mu_k I\right) s = -J^T R, \quad \mu_k > 0$$
- System above are normal equations for
$$\min_{s\in\mathbb{R}^n} \frac{1}{2}\left\| \begin{bmatrix} J \\ \sqrt{\mu_k} I_n \end{bmatrix} s + \begin{bmatrix} R \\ 0 \end{bmatrix} \right\|_2^2$$

Use QR decomposition to solve for s.

Goal: Parameterize Solution Set $\mathcal{M}$

- Assume $R(p^*) = 0$, rank $J(p) = r < n$ for p in neighborhood of p_*. Want characterization of solution manifold, locally.
- Linear case: Can parameterize $\mathcal{M}$ by a mapping
$$\mathbb{R}^{n-r} \ni q \mapsto p^* + V_{n-r}\, q.$$
- General case: Want to find a mapping $B : W \subset \mathbb{R}^{n-r} \to \mathbb{R}^n$ such that for some neighborhood $U \subset \mathbb{R}^n$ of p^*,
$$\mathcal{M} \cap U = \{B(q) \;:\; q \in W\}.$$

Constant Rank Theorem [1]

Let $U \subset \mathbb{R}^n$ be open, $R : U \to \mathbb{R}^m$ be continuously differentiable.
If Jacobian R has constant rank $r < n$ in neighborhood U of p, there is local coord. system g at p and local coord. system h at $R(p)$ s.t.
$$h^{-1} R g(x_1, \ldots, x_n) = (x_1, \ldots, x_r, 0, \ldots, 0).$$

Local Characterization of the Solution Set

Assumption 1. $R : \mathbb{R}^n \mapsto \mathbb{R}^m$ cont. differentiable, rank $J(p) = r < n$ in a neighborhood U of $p^* \in \mathcal{M}$,
Assumption 2. $R(p) = R(p^*)$ for any $p \in \mathcal{M} \cap U$.

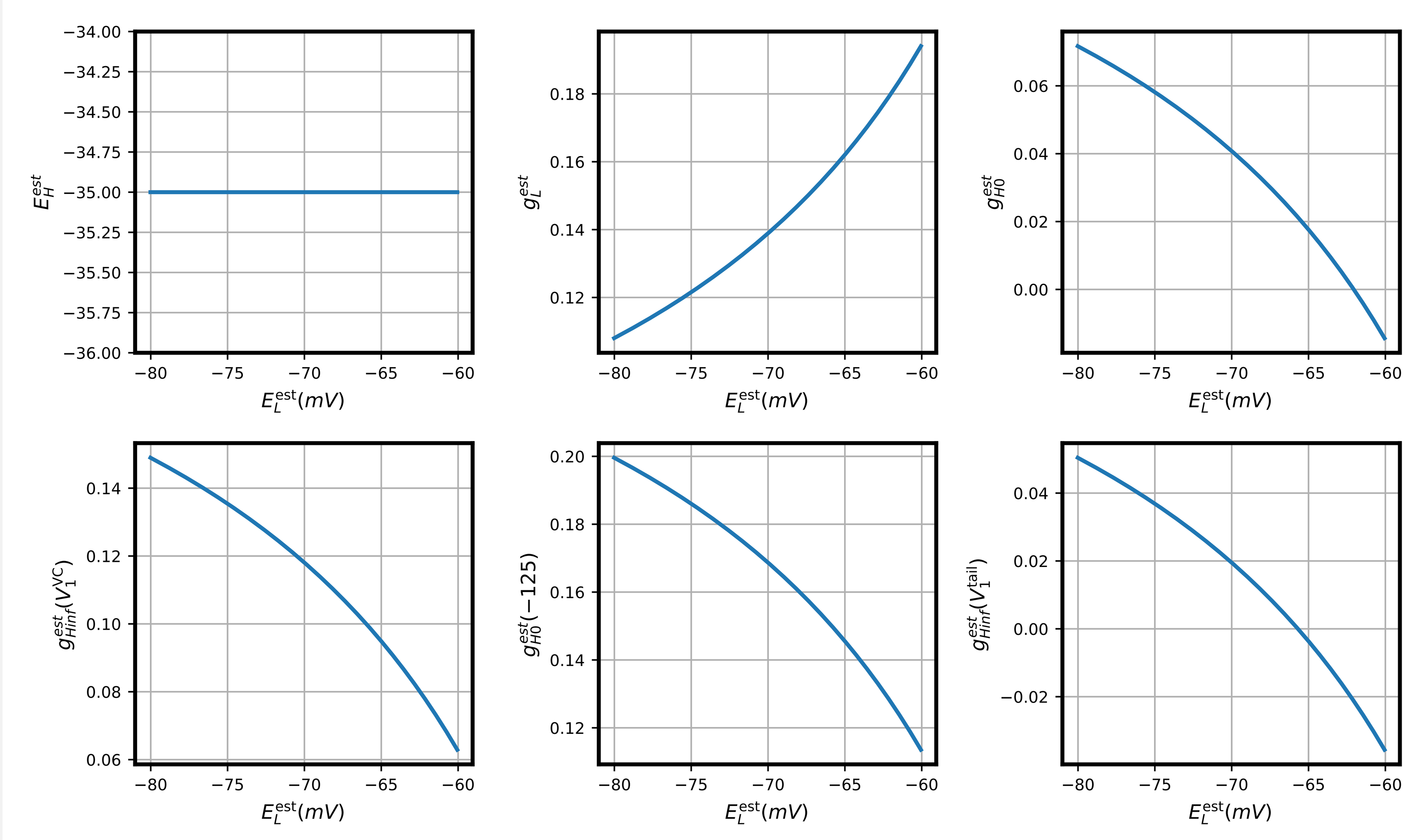
From Constant Rank Theorem and Assumptions 1 and 2, can parameterize $\mathcal{M}$ in a neighborhood of p^* by a mapping
$$B(q_{r+1}, \ldots, q_n) = g\left((h^{-1}R(p^*))_1, \ldots, (h^{-1}R(p^*))_r, q_{r+1}, \ldots, q_n \right).$$

HCN Neuron Model

- Constant voltage V, given $h(t_{\text{init}}) = h_\infty(V_{\text{ref}})$, $h_\infty(V)$, $\tau_H(V)$:
$$I(t) = -g_L\big(V - E_L\big) - \bar{g}_H h(t)\big(V - E_H\big), \qquad t \in [t_{\text{init}}, t_{\text{final}}]$$
$$\frac{d}{dt} h(t) = \frac{h_\infty(V) - h(t)}{\tau_H(V)}, \qquad t \in [t_{\text{init}}, t_{\text{final}}].$$
- Analytic solution:
$$I(t) = g_L(V - E_L) + \Big(g_{H,\infty}(V_{\text{ref}}) + \big(g_{H,\infty}(V) - g_{H,\infty}(V_{\text{ref}})\big) \times \Big(1 - e^{-(t - t_{\text{init}})/\tau_H(V)}\Big) \Big) \big(V - E_H\big)$$
- Apply voltages $V_c^1, \ldots, V_c^5$ with $V_{ref}^1 = -60[mV]$ and $V_{\text{tail}}^1, \ldots, V_{\text{tail}}^3$ with $V_{ref}^2 = -125[mV]$ and measure current.
- Estimate parameters $E_L, E_H, g_L, g_{H,\infty}(V_{\text{ref}}^1), g_{H,\infty}(V_c^1), \ldots, g_{H,\infty}(V_c^5), g_{H,\infty}(V_{\text{ref}}^2), g_{H,\infty}(V_{\text{tail}}^1), g_{H,\infty}(V_{\text{tail}}^2), g_{H,\infty}(V_{\text{tail}}^3)$.

Solution Manifold in HCN Neuron Model

- Use synthetic current data to estimate parameters in least squares using Levenberg-Marquardt.
- Have $m = 13{,}923$ measurements, $n = 13$ parameters.
- Jacobian rank 1-deficient with $r = 12$.
- Subset selection algorithm described in [2, Sec 5.5.7] determines E_L as least identifiable parameter.
- Take initial E_L on a grid $[-80, -79.95, \ldots -60.05, -60]$ and fix initial values of other parameters.



Projections of a solution manifold

Future Work

Find computational framework to characterize solution set in rank-deficient least squares problems.

References and Acknowledgments

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