Trajectory-based optimization

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Using the maximum principle

Recall that for deterministic dynamics $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u})$ and cost rate $\ell(\mathbf{x}, \mathbf{u})$ the optimal state-control-costate trajectory $(\mathbf{x}(\cdot), \mathbf{u}(\cdot), \boldsymbol{\lambda}(\cdot))$ satisfies

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{f}(\mathbf{x}, \mathbf{u}) \\ -\dot{\boldsymbol{\lambda}} &= \ell_{\mathbf{x}}(\mathbf{x}, \mathbf{u}) + \mathbf{f}_{\mathbf{x}}(\mathbf{x}, \mathbf{u})^{\mathsf{T}} \boldsymbol{\lambda} \\ \mathbf{u} &= \arg\min_{\widetilde{\mathbf{u}}} \left\{ \ell(\mathbf{x}, \widetilde{\mathbf{u}}) + \mathbf{f}(\mathbf{x}, \widetilde{\mathbf{u}})^{\mathsf{T}} \boldsymbol{\lambda} \right\} \end{aligned}$$

with $\mathbf{x}(0)$ given and $\boldsymbol{\lambda}(T) = \frac{\partial}{\partial \mathbf{x}} q_{\mathcal{T}}(\mathbf{x}(T))$. Solving this boundary-value ODE problem numerically is a trajectory-based method.

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We can also use the fact that, if $(\mathbf{x}(\cdot), \boldsymbol{\lambda}(\cdot))$ satisfies the ODE for some $\mathbf{u}(\cdot)$ which is not a minimizer of the Hamiltonian $H(\mathbf{x}, \mathbf{u}, \boldsymbol{\lambda}) = \ell(\mathbf{x}, \mathbf{u}) + \mathbf{f}(\mathbf{x}, \mathbf{u})^{\mathsf{T}} \boldsymbol{\lambda}$, then the gradient of the total cost J is given by

$$\begin{aligned} J(\mathbf{x}(\cdot), \mathbf{u}(\cdot)) &= q_{\mathcal{T}}(\mathbf{x}(T)) + \int_0^T \ell(\mathbf{x}(t), \mathbf{u}(t))\, dt \\ \frac{\partial J}{\partial \mathbf{u}(t)} &= H_{\mathbf{u}}(\mathbf{x}, \mathbf{u}, \boldsymbol{\lambda}) = \ell_{\mathbf{u}}(\mathbf{x}, \mathbf{u}) + \mathbf{f}_{\mathbf{u}}(\mathbf{x}, \mathbf{u})^{\mathsf{T}} \boldsymbol{\lambda} \end{aligned}$$

Thus we can perform gradient descent on J with respect to $\mathbf{u}(\cdot)$

Compact representations

Given the current $\mathbf{u}(\cdot)$, each step of the algorithm involves computing $\mathbf{x}(\cdot)$ by integrating forward in time starting with the given $\mathbf{x}(0)$, then computing $\boldsymbol{\lambda}(\cdot)$ by integrating backward in time starting with $\boldsymbol{\lambda}(T) = \frac{\partial}{\partial \mathbf{x}} q_T(\mathbf{x}(T))$.

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One way to implement the above methods is to discretize the time axis and represent $(\mathbf{x}, \mathbf{u}, \boldsymbol{\lambda})$ independently at each time step. This may be inefficient because the values at nearby time steps are usually very similar, thus it is a waste to represent/optimize them independently.

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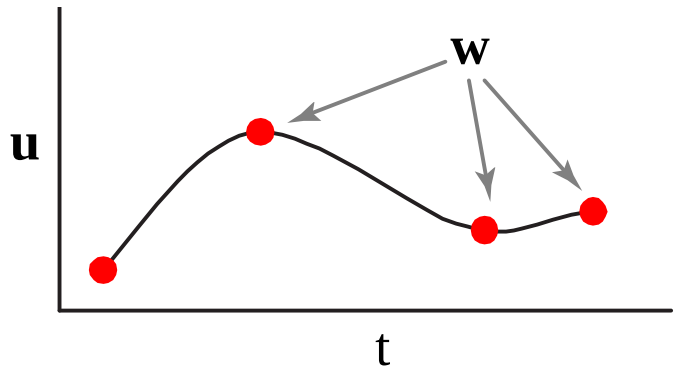
Instead we can splines, Legendre or Chebyshev polynomials, etc.

$$\mathbf{u}(t) = \mathbf{g}(t, \mathbf{w})$$

Gradient:

$$\frac{\partial J}{\partial \mathbf{w}} = \int_0^T \mathbf{g}_{\mathbf{w}}(t, \mathbf{w})^{\mathsf{T}} \frac{\partial J}{\partial \mathbf{u}(t)} dt$$



Space-time constraints

We can also minimize the total cost J as an explicit function of the (parameterized) state-control trajectory:

$$\begin{aligned} \mathbf{x}(t) &= \mathbf{h}(t, \mathbf{v}) \\ \mathbf{u}(t) &= \mathbf{g}(t, \mathbf{w}) \end{aligned}$$

We have to make sure that the state-control trajectory is consistent with the dynamics $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u})$. This yields a constrained optimization problem:

$$\min_{\mathbf{v},\mathbf{w}} \left\{ q_{\mathcal{T}}(\mathbf{h}(T, \mathbf{v})) + \int_0^T \ell(\mathbf{h}(t, \mathbf{v}), \mathbf{g}(t, \mathbf{w}))\, dt \right\}$$

$$s.t. \quad \frac{\partial \mathbf{h}(t, \mathbf{v})}{\partial t} = \mathbf{f}(\mathbf{h}(t, \mathbf{v}), \mathbf{g}(t, \mathbf{v})), \quad \forall t \in [0, T]$$

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In practice we cannot impose the contraint for all t, so instead we choose a finite set of points $\{t_k\}$ where the constraint is enforced. The same points can also be used to approximate $\int \ell$. There may be no feasible solution (depending on $\mathbf{h}, \mathbf{g}$) in which case we have to live with constraint violations.

This requires no knowledge of optimal control (which may be why it is popular:)

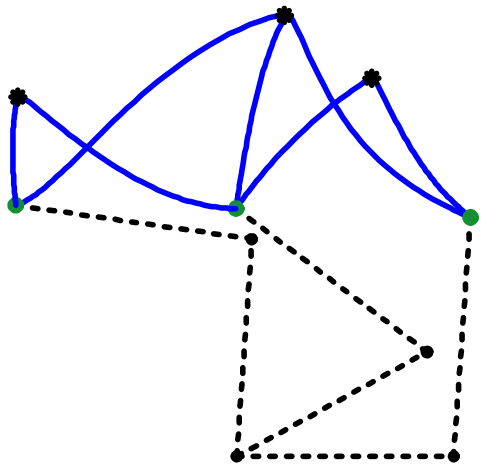
Second-order methods

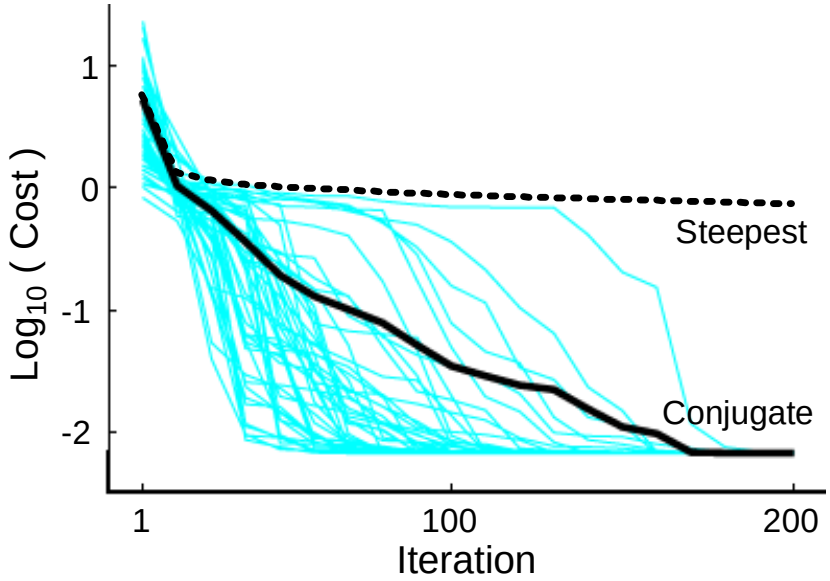
More efficient methods (DDP, iLQG) can be constructed by using the Bellman equations locally. Initialize with some open-loop control $\mathbf{u}^{(0)}(\cdot)$, and repeat:

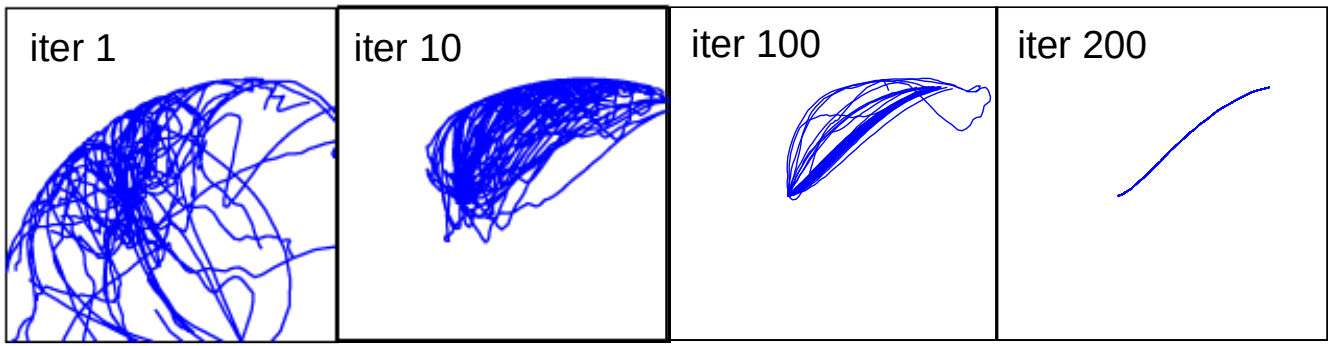
1. Compute the state trajectory $\mathbf{x}^{(n)}(\cdot)$ corresponding to $\mathbf{u}^{(n)}(\cdot)$.
2. Construct a time-varying linear (iLQG) or quadratic (DDP) approximation to the function $\mathbf{f}$ around $\mathbf{x}^{(n)}(\cdot), \mathbf{u}^{(n)}(\cdot)$, which gives the local dynamics in terms of the state and control deviations $\delta\mathbf{x}(\cdot), \delta\mathbf{u}(\cdot)$. Also construct quadratic approximations to the costs ℓ and $q_{\mathcal{T}}$.
3. Compute the locally-optimal cost-to-go $v^{(n)}(\delta\mathbf{x}, t)$ as a quadratic in $\delta\mathbf{x}$. In iLQG this is exact (because the local dynamics are linear and the cost is quadratic) while in DDP this is approximate.
4. Compute the locally-optimal linear feedback control law in the form $\boldsymbol{\pi}^{(n)}(\delta\mathbf{x}, t) = \mathbf{c}(t) - L(t)\,\delta\mathbf{x}$.
5. Apply $\boldsymbol{\pi}^{(n)}$ to the local dynamics (i.e. integrate forward in time) to compute the state-control modification $\delta\mathbf{x}^{(n)}(\cdot), \delta\mathbf{u}^{(n)}(\cdot)$, and set $\mathbf{u}^{(n+1)}(\cdot) = \mathbf{u}^{(n)}(\cdot) + \delta\mathbf{u}^{(n)}(\cdot)$. This requires linesearch to avoid jumping outside the region where the local approximation is valid.

Numerical comparison

	Conj.	ODE	DDP
time(s)	**5.9**	**1.25**	**0.61**







Gradient descent

The directional derivative of $f(\mathbf{x})$ at $\mathbf{x}_0$ in direction $\mathbf{v}$ is

$$D_{\mathbf{v}}[f](\mathbf{x}_0) = \left. \frac{df(\mathbf{x}_0 + \varepsilon \mathbf{v})}{d\varepsilon} \right|_{\varepsilon=0}$$

Let $\mathbf{x}(\varepsilon) = \mathbf{x}_0 + \varepsilon \mathbf{v}$. Then $f(\mathbf{x}_0 + \varepsilon \mathbf{v}) = f(\mathbf{x}(\varepsilon))$ and the chain rule yields

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where $\mathbf{g}$ denotes the gradient of f.

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Theorem (steepest ascent direction)

The maximum of $D_{\mathbf{v}}[f](\mathbf{x}_0)$ s.t. $\|\mathbf{v}\| = 1$ is achieved when $\mathbf{v}$ is parallel to $\mathbf{g}(\mathbf{x}_0)$.

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Algorithm (gradient descent)

Set $\mathbf{x}_{k+1} = \mathbf{x}_k - \beta_k \mathbf{g}(\mathbf{x}_k)$ where β_k is the step size. The optimal step size is

$$\beta_k^* = \arg\min_{\beta_k} f(\mathbf{x}_k - \beta_k \mathbf{g}(\mathbf{x}_k))$$

Line search

Most optimization methods involve an inner loop which seeks to minimize (or sufficiently reduce) the objective function constrained to a line: $f(\mathbf{x} + \varepsilon \mathbf{v})$, where $\mathbf{v}$ is such that a reduction in f is always possible for sufficiently small ε, unless f is already at a local minimum. In gradient descent $\mathbf{v} = -\mathbf{g}(\mathbf{x})$; other choices are possible (see below) as long as $\mathbf{v}^{\mathsf{T}} \mathbf{g}(\mathbf{x}) \leq 0$.

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This is called *linesearch*, and can be done in different ways:

1. Backtracking: try some ε, if $f(\mathbf{x} + \varepsilon \mathbf{v}) > f(\mathbf{x})$ reduce ε and try again.
2. Bisection: attempt to minimize $f(\mathbf{x} + \varepsilon \mathbf{v})$ w.r.t. ε using a bisection method.
3. Polysearch: attempt to minimize $f(\mathbf{x} + \varepsilon \mathbf{v})$ by fitting quadratic or cubic polynomials in ε, finding the minimum analytically, and iterating.

Exact minimization w.r.t. ε is often a waste of time because for $\varepsilon \neq 0$ the current search direction may no longer be a descent direction.

Sufficient reduction in f is defined relative to the local model (linear or quadratic). This is known as the Armijo-Goldstein condition; the Wolfe condition (which also involves the gradient) is more complicated.

Chattering

If $\mathbf{x}_{k+1}$ is a (local) minimum of f in the search direction $\mathbf{v}_k = -\mathbf{g}(\mathbf{x}_k)$, then $D_{\mathbf{v}_k}[f](\mathbf{x}_{k+1}) = 0 = \mathbf{v}_k^{\mathsf{T}} \mathbf{g}(\mathbf{x}_{k+1})$, and so if we use $\mathbf{v}_{k+1} = -\mathbf{g}(\mathbf{x}_{k+1})$ as the next search direciton, we have $\mathbf{v}_{k+1}$ orthogonal to $\mathbf{v}_k$. Thus gradient descent with exact line search (i.e. steepest descent) makes a 90 deg turn at each iteration, which causes chattering when the function has a long oblique valey.

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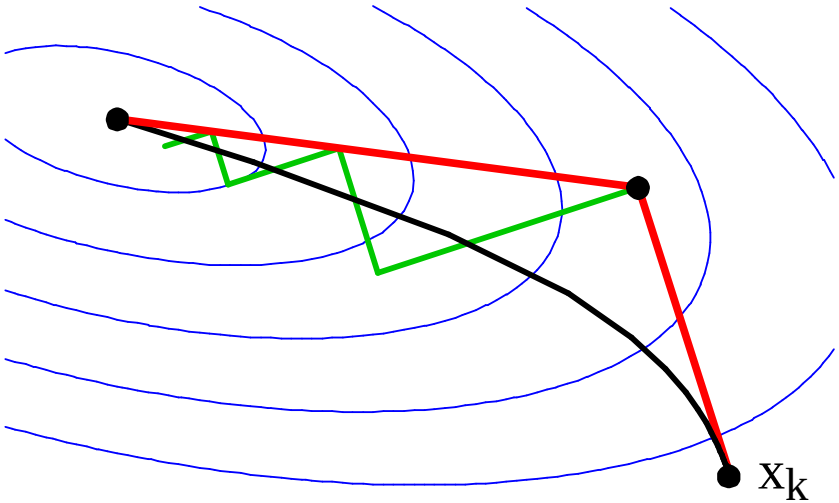

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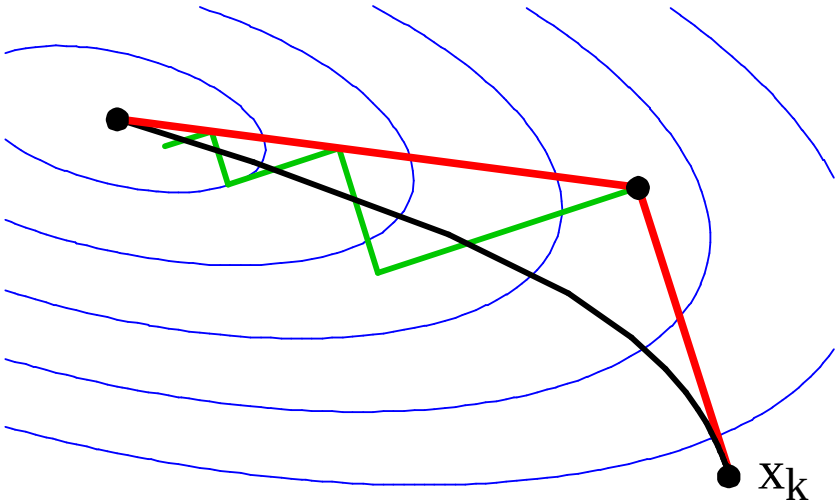

Key to developing more efficient methods is to anticipate how the gradient will rotate as we move along the current search direction.

Newton's method

Theorem

If all you have is a hammer, then everything looks like a nail.

Corollary

If all you can optimize is a quadratic, then every function looks like a quadratic.

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Taylor-expand $f(\mathbf{x})$ around the current solution $\mathbf{x}_k$ up to 2nd order:

$$f(\mathbf{x}_k + \boldsymbol{\varepsilon}) = f(\mathbf{x}_k) + \boldsymbol{\varepsilon}^T \mathbf{g}(\mathbf{x}_k) + \frac{1}{2} \boldsymbol{\varepsilon}^T H(\mathbf{x}_k) \boldsymbol{\varepsilon} + o\left(\boldsymbol{\varepsilon}^3\right)$$

where $\mathbf{g}(\mathbf{x}_k)$ and $H(\mathbf{x}_k)$ are the gradient and Hessian of f at $\mathbf{x}_k$:

$$\mathbf{g}(\mathbf{x}_k) \triangleq \left. \frac{\partial f}{\partial \mathbf{x}} \right|_{\mathbf{x}=\mathbf{x}_k} \qquad H(\mathbf{x}_k) \triangleq \left. \frac{\partial^2 f}{\partial \mathbf{x} \partial \mathbf{x}^T} \right|_{\mathbf{x}=\mathbf{x}_k}$$

Assuming H is (symmetric) positive definite, the next solution is

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \arg\min_{\boldsymbol{\varepsilon}} \left\{ \boldsymbol{\varepsilon}^T \mathbf{g} + \frac{1}{2} \boldsymbol{\varepsilon}^T H \boldsymbol{\varepsilon} \right\} = \mathbf{x}_k - H^{-1} \mathbf{g}$$

Stabilizing Newton's method

For *convex* functions the Hessian H is always s.p.d, so the above method converges (usually quickly) to the global minimum. In reality however most functions we want to optimize are non-convex, which causes two problems:

1. H may be singular, which means that $\mathbf{x}_{k+1} = \mathbf{x}_k - H^{-1}\mathbf{g}$ will take us all the way to infinity.
2. H may have negative eigenvalues, which measn that (even if $\mathbf{x}_{k+1}$ is finite) we end up finding saddle points – minimum in some directions, maximum in other directions.

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These problems can be avoided in two general ways:

1. Trust region: minimize $\boldsymbol{\varepsilon}^{\mathsf{T}}\mathbf{g} + \frac{1}{2}\boldsymbol{\varepsilon}^{\mathsf{T}}H\boldsymbol{\varepsilon}$ s.t. $\|\boldsymbol{\varepsilon}\| \leq r$, where r is adapted over iterations. The minimization is usually done approximately.
2. Convexification/linearsearch: replace H with $H + \lambda I$, and/or use backtracking linesearch starting at the Newton point. When λ is large, $\mathbf{x}_k - (H + \lambda I)^{-1}\mathbf{g} \approx \mathbf{x}_k - \lambda^{-1}\mathbf{g}$, which is gradient descent with step λ^{-1}. The Levenberg-Marquardt method adapts λ over iterations.

Relation to linear solvers

The quadratic function

$$f(\mathbf{x}_k + \boldsymbol{\varepsilon}) = f(\mathbf{x}_k) + \boldsymbol{\varepsilon}^{\mathsf{T}} \mathbf{g}(\mathbf{x}_k) + \frac{1}{2} \boldsymbol{\varepsilon}^{\mathsf{T}} H(\mathbf{x}_k) \boldsymbol{\varepsilon}$$

is minimized when the gradient w.r.t $\boldsymbol{\varepsilon}$ vanishes, i.e. when

$$H\boldsymbol{\varepsilon} = -\mathbf{g}$$

When H is s.p.d, one can use the conjugate-gradient method for solving linear equations to do numerical optimization.

The set of vectors $\{\mathbf{v}_k\}_{k=1\cdots n}$ are conjugate if they satisfy $\mathbf{v}_i^{\mathsf{T}} H \mathbf{v}_j = 0$ for $i \neq j$. These are good search directions because they yield exact minimization of an n-dimensional quadratic in n iterations (using exact linesearch). Such a set can be constructed using Lanczos iteration:

$$s_{k+1}\mathbf{v}_{k+1} = (H - \alpha_k I)\mathbf{v}_k - s_k \mathbf{v}_{k-1}$$

where s_{k+1} is such that $\|\mathbf{v}_{k+1}\| = 1$, and $\alpha_k = \mathbf{v}_k^{\mathsf{T}} H \mathbf{v}_k$. Note that access to H is not required; all we need to be able to compute is $H\mathbf{v}$.

Non-linear least squares

Many optimization problems are in the form

$$f(\mathbf{x}) = \frac{1}{2} \|\mathbf{r}(\mathbf{x})\|^2$$

where $\mathbf{r}(\mathbf{x})$ is a vector of "residuals". Define the Jacobian of the residuals:

$$J(\mathbf{x}) = \frac{\partial \mathbf{r}(\mathbf{x})}{\partial \mathbf{x}}$$

Then the gradient and Hessian of f are

$$\begin{aligned} \mathbf{g}(\mathbf{x}) &= J(\mathbf{x})^\mathsf{T} \mathbf{r}(\mathbf{x}) \\ H(\mathbf{x}) &= J(\mathbf{x})^\mathsf{T} J(\mathbf{x}) + \frac{\partial J(\mathbf{x})}{\partial \mathbf{x}} \times \mathbf{r}(\mathbf{x}) \end{aligned}$$

We can omit the last term and obtain the Gauss-Netwon approximation:

$$H(\mathbf{x}) \approx J(\mathbf{x})^\mathsf{T} J(\mathbf{x})$$

Then Newton's method (with stabilization) becomes

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \left(J_k^\mathsf{T} J_k + \lambda_k I\right)^{-1} J_k^\mathsf{T} \mathbf{r}_k$$