Numerical Optimization

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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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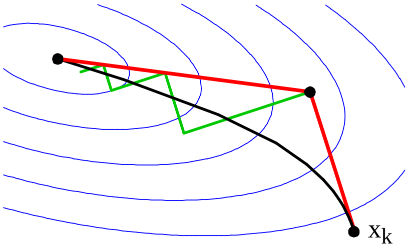

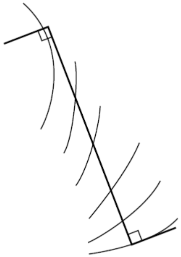

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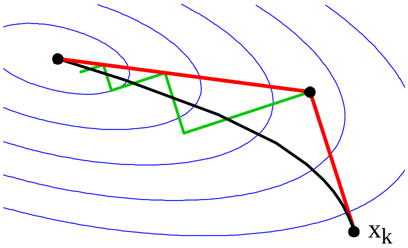

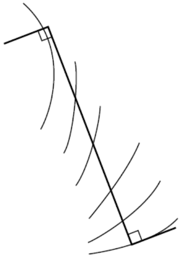

Key to developing more efficient methods is to anticipate how the gradient will rotate as we move along the current search direction.

Newton's method

Theorem

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

Corollary

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

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

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

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

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

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

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

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

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:

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

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

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