Non-convex optimization

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Strongly Convex

Objective function

 $\min_{x \in \mathbb{R}^n} f(x),$



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Assumptions

Gradient Lipschitz continuous

$$f(y) \le f(x) + \nabla f(x)(y-x) + \frac{L}{2}(y-x)^2$$

Strongly convex

 $f(y) \geq f(x) + \nabla f(x)(y-x) + \tfrac{\mu}{2}(y-x)^2$



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Randomized coordinate descent

$$E[f(x^{t+1}) - f(x^t)] \le (1 - \frac{\mu}{nL})[f(x^t) - f(x^*)]$$



Non-strongly Convex optimization

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$$f(y) \le f(x) + \nabla f(x)(y-x) + \frac{L}{2}(y-x)^2$$

Convergence rate

$$f(x^{t}) - f(x^{*}) = O(1/t).$$

Compared to the strongly convex convergence rate

$$F(x^{t}) - f(x^{*}) = O(\rho^{t})$$
$$E[f(x^{t+1}) - f(x^{t})] \le (1 - \frac{\mu}{nL})[f(x^{t}) - f(x^{*})]$$



Non-strongly Convex optimization

Definition 2 (Restricted secant inequality – $RSI(\nu)$). A function $f(x) : \mathbb{R}^n \to \mathbb{R}$ satisfies the restricted secant inequality (RSI) with constant $\nu > 0$ if it is differentiable and obeys

$$\langle \nabla f(x) - \nabla f(x_{\text{prj}}), x - x_{\text{prj}} \rangle \ge \nu \|x - x_{\text{prj}}\|^2, \tag{7}$$



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Restricted secant inequality

$$\langle \nabla f(x) - \nabla f(x_{\mathrm{prj}}), x - x_{\mathrm{prj}} \rangle \ge \nu \|x - x_{\mathrm{prj}}\|^2.$$

Randomized coordinate descent

$$E[f(x^{t+1}) - f(x^t)] \le (1 - \frac{v}{nL})[f(x^t) - f(x^*)]$$



Invex functions (a generalization of convex function)

Objective function

 $\min_{x\in\mathbb{R}^n} f(x),$

Assumptions

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$$f(y) \le f(x) + \nabla f(x)(y-x) + \frac{L}{2}(y-x)^2$$

Polyak [1963]

 $||\nabla f(x)||^2 \ge 2\mu (f(x) - f^*).$

This inequality simply requires that the gradient grows faster than a linear function as we move away from the optimal function value.



Invex function (one global minimum)

Invex functions (a generalization of convex function)

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Polyak [1963] - for invex functions where this holds $||\nabla f(x)||^2 \geq 2\mu (f(x) - f^*),$

Randomized coordinate descent

$$E[f(x^{t+1}) - f(x^t)] \le (1 - \frac{\mu}{nL})[f(x^t) - f(x^*)]$$



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$$E[f(x^{t+1}) - f(x^t)] \le (1 - \frac{\mu}{nL})[f(x^t) - f(x^*)]$$



Venn diagram







Strategy 1: local optimization of the non-convex function



Assumptions for local non-convex optimization

Lipschitz continuous

$$f(y) \le f(x) + \nabla f(x)(y-x) + \frac{L}{2}(y-x)^2$$

Locally convex

$$||\nabla f(x)||^2 \ge 2\mu (f(x) - f^*).$$



Local randomized coordinate descent $E[f(x^{t+1}) - f(x^t)] \le (1 - \frac{\mu}{nL})[f(x^t) - f(x^*)]$

Strategy 1: local optimization of the non-convex function

All convex functions rates apply.



Strategy 1: local optimization of the non-convex function

Issue: dealing with saddle points



Strategy 2: Global optimization of the non-convex function

Issue: Exponential number of saddle points

Local non-convex optimization

- Gradient Descent
 - Difficult to define a proper step size

 $x^{t+1} = x^t - \alpha \nabla f(x^t)$

Newton method

- Newton method solves the slowness problem by rescaling the gradients in each direction with the inverse of the corresponding eigenvalues of the hessian
- \circ ~ can result in moving in the wrong direction (negative eigenvalues)

 $x^{t+1} = x^t - \nabla f(x^t) \nabla^2 f(x^t)^{-1}$

Saddle-Free Newton's method

 rescales gradients by the absolute value of the inverse Hessian and the Hessian's Lanczos vectors.



Local non-convex optimization

- Random stochastic gradient descent
 - Sample noise *r* uniformly from unit sphere
 - Escapes saddle points but step size is difficult to determine

 $x^{t+1} = x^t - \alpha [\nabla f(x^t) + r]$

• Cubic regularization [Nesterov 2006]

Gradient Lipschitz continuous

$$f(y) \leq f(x) + \nabla f(x)(y-x) + \frac{L}{2}(y-x)^2$$

Hessian Lipschitz continuous

$$f(x^{t+1}) \le f(x^t) + \nabla f(x^t)(x^{t+1} - x^t) + \frac{\nabla^2 f(x^t)}{2}(x^{t+1} - x^t)^2 + \frac{M}{6}|x^{t+1} - x^t|^3$$

Then there exist constants ϵ , $\delta > 0$ such that whenever a point x_i appears to be in a set $Q = \{x : ||x - \bar{x}|| \le \epsilon, f(x) \ge f(\bar{x})\}$ (for instance, if $x_i = \bar{x}$), then the next point x_{i+1} leaves the set Q:

$$f(x_{i+1}) \le f(\bar{x}) - \delta.$$



Local non-convex optimization

- Random stochastic gradient descent
 - Sample noise *r* uniformly from unit sphere
 - Escapes saddle points but step size is difficult to determine

$$x^{t+1} = x^t - \alpha [\nabla f(x^t) + r]$$

- Momentum
 - can help escape saddle points (rolling ball)

$$v^{t+1} = \rho v^t - \alpha \nabla f(x^t)$$

$$x^{t+1} = x^t + v^{t+1}$$



Global non-convex optimization

- Matrix completion problem [De Sa et al. 2015] minimize $\mathbf{E} \left[\left\| \tilde{A} - X \right\|_{F}^{2} \right]$ subject to $X \in \mathbb{R}^{n \times n}$, rank $(X) \le p, X \succeq 0$,
- Applications (usually for datasets with missing data)
 - matrix completion
 - Image reconstruction
 - recommendation systems.

Global non-convex optimization

- Matrix completion problem [De Sa et al. 2015] minimize $\mathbf{E} \left[\left\| \tilde{A} - X \right\|_{F}^{2} \right]$ subject to $X \in \mathbb{R}^{n \times n}$, rank $(X) \leq p, X \succeq 0$,
- Reformulate it as (unconstrained non-convex problem) minimize $\mathbf{E} \left[\|\tilde{A} - YY^T\|_F^2 \right]$ subject to $Y \in \mathbb{R}^{n \times p}$

• Gradient descent

$$Y_{k+1} = Y_k + \alpha_k \left(\tilde{A}_k - Y_k Y_k^T \right) Y_k.$$

Global non-convex optimization

• Reformulate it as (unconstrained non-convex problem) minimize $\mathbf{E} \left[\|\tilde{A} - YY^T\|_F^2 \right]$. subject to $Y \in \mathbb{R}^{n \times p}$

• Gradient descent

 $Y_{k+1} = Y_k + \alpha_k \left(\tilde{A}_k - Y_k Y_k^T \right) Y_k.$

• Using the Riemannian manifold, we can derive the following

 $Y_{k+1} = \left(I + \eta_k \tilde{A}_k\right) Y_k.$

• This widely-used algorithm converges globally, using only random initialization

Convex relaxation of non-convex functions optimization

- Convex Neural Networks [Bengio et al. 2006]
 - Single-hidden layer network

 $L(x, y) = \frac{1}{2} ||f(x, y) - b||^2$

$$f(x, y) = y \cdot g(Ax)$$



original neural networks non-convex problem

Convex relaxation of non-convex functions optimization

- Convex Neural Networks [Bengio et al. 2006]
 - Single-hidden layer network

 $L(x, y) = \frac{1}{2} ||f(x, y) - b||^2$

$$f(x, y) = y \cdot g(Ax)$$

• Use alternating minimization

$$L_{c}(x) = \frac{1}{2} ||f_{c}(x) - b||^{2} \qquad f_{c}(x) = h(v) \cdot x$$
$$L_{h}(v) = \frac{1}{2} ||h(v) - f_{c}(x)||^{2} \qquad h(v) = g(Av)$$

• Potential issues with the activation function

Bayesian optimization (global non-convex optimization)

- Typically used for finding optimal parameters
 - Determining the step size of # hidden layers for neural networks
 - The parameter values are bounded ?
- Other methods include sampling the parameter values random uniformly
 - Grid-search



Bayesian optimization (global non-convex optimization)

- Fit Gaussian process on the observed data (purple shade)
 - Probability distribution on the function values



Bayesian optimization (global non-convex optimization)

- Fit Gaussian process on the observed data (purple shade)
 - Probability distribution on the function values
- Acquisition function (green shade)
 - a function of
 - the objective value (exploitation) in the Gaussian density function; and
 - the uncertainty in the prediction value (exploration).



Bayesian optimization

- Slower than grid-search with low level of smoothness (illustrate)
- Faster than grid-search with high level of smoothness (illustrate)



Bayesian optimization

- Slower than grid-search with low level of smoothness (illustrate)
- Faster than grid-search with high level of smoothness (illustrate)

Improves error from $O(1/t^{1/d})$ to $O(1/t^{v/d})$

Grid-search

Bayesian optimization



Bayesian optimization

- Slower than grid-search with low level of smoothness (illustrate)
- Faster than grid-search with high level of smoothness (illustrate)

Improves error from $O(1/t^{1/d})$ to $O(1/t^{\sqrt{d}})$

Grid-search

Bayesian optimization



Summary

Non-convex optimization

- Strategy 1: Local non-convex optimization
 - Convexity convergence rates apply
 - Escape saddle points using, for example, cubic regularization and saddle-free newton update
- Strategy 2: Relaxing the non-convex problem to a convex problem
 - Convex neural networks
- Strategy 3: Global non-convex optimization
 - Bayesian optimization
 - Matrix completion