Beyond SG: Noise Reduction and Second-Order Methods

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Outline

What have we learned about SG?

Assumption $\langle L/c \rangle$

The objective function $F : \mathbb{R}^d \to \mathbb{R}$ is

- *c-strongly convex ($\Rightarrow$ unique minimizer) and*
- *L-smooth (i.e., ∇F is Lipschitz continuous with constant L).*

Theorem SG (sublinear convergence)

Under Assumption $\langle L/c \rangle$ and $\mathbb{E}_{\xi_k}[\|g(w_k, \xi_k)\|_2^2] \leq M + \mathcal{O}(\|\nabla F(w_k)\|_2^2)$,

$$w_{k+1} \leftarrow w_k - \alpha_k g(w_k, \xi_k)$$

yields

$$\alpha_k = \frac{1}{L} \qquad \Longrightarrow \mathbb{E}[F(w_k) - F_*] \to \frac{M}{2c};$$

$$\alpha_k = \mathcal{O}\left(\frac{1}{k}\right) \qquad \Longrightarrow \mathbb{E}[F(w_k) - F_*] = \mathcal{O}\left(\frac{(L/c)(M/c)}{k}\right).$$

(*Let's assume unbiased gradient estimates; see paper for more generality.)

Illustration

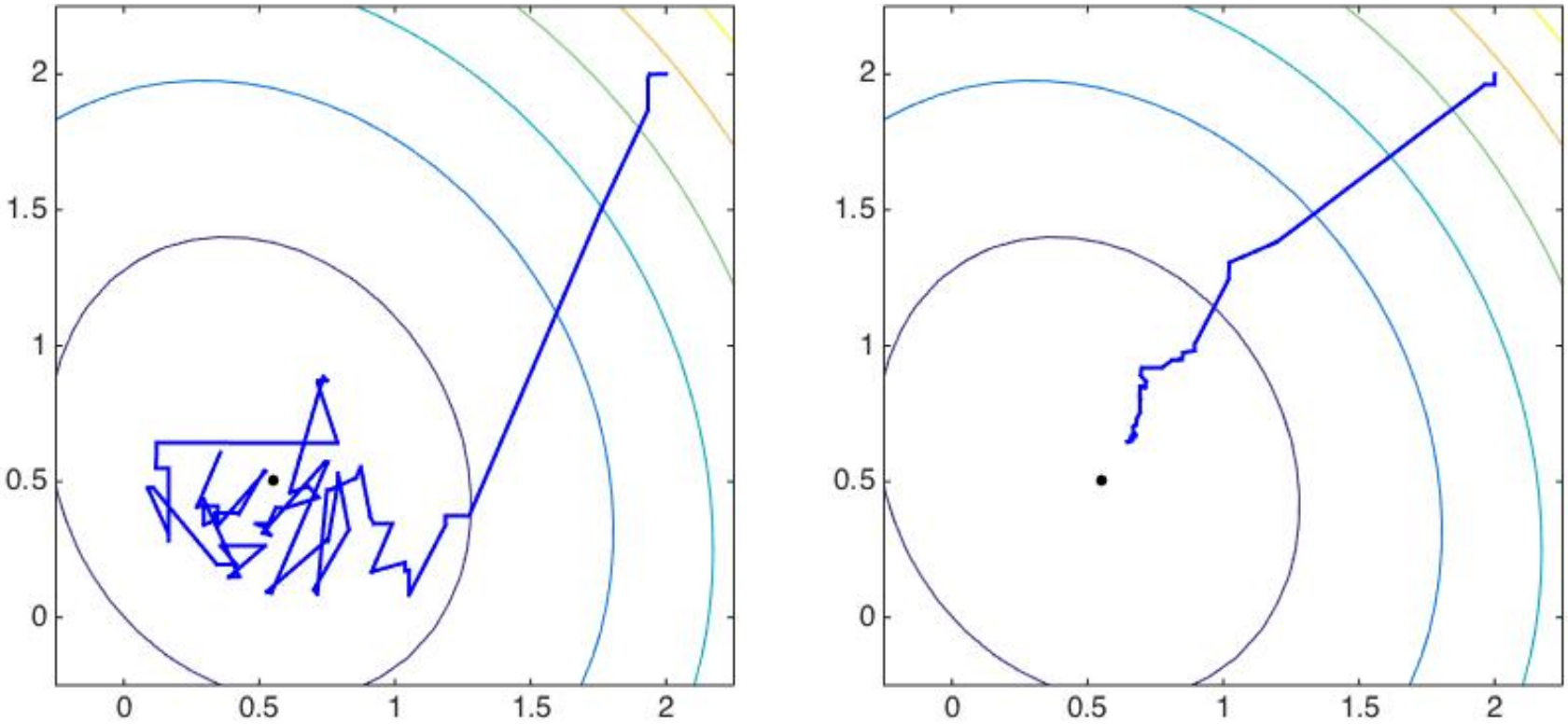
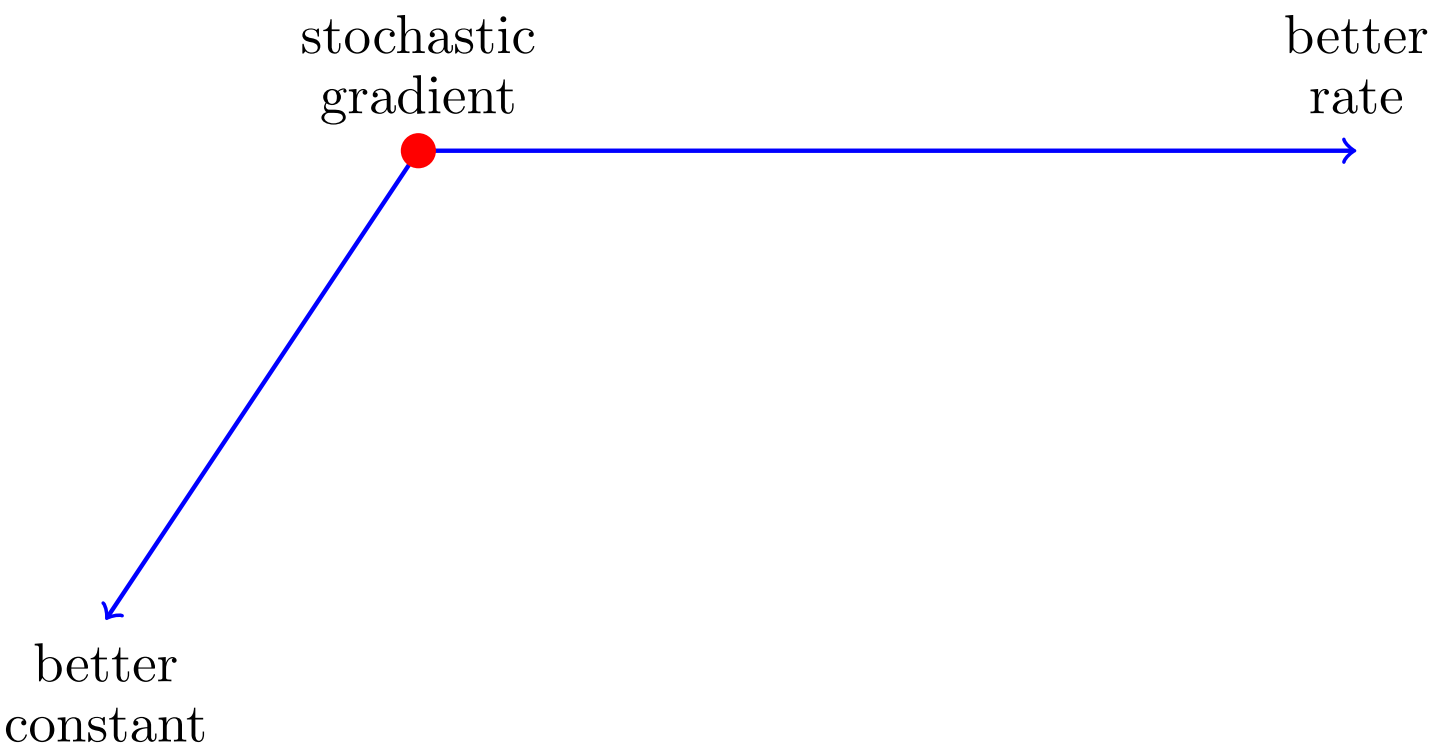
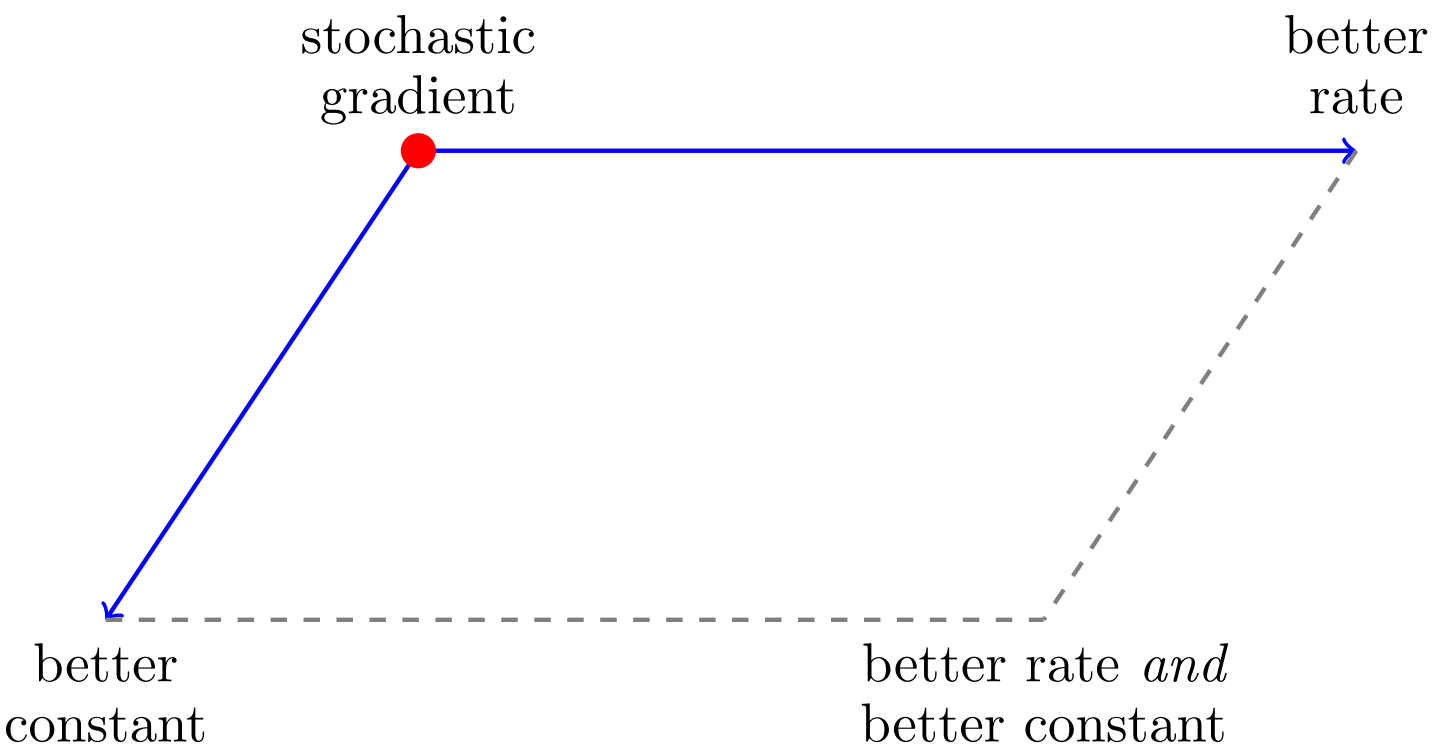


Figure: SG run with a fixed stepsize (left) vs. diminishing stepsizes (right)

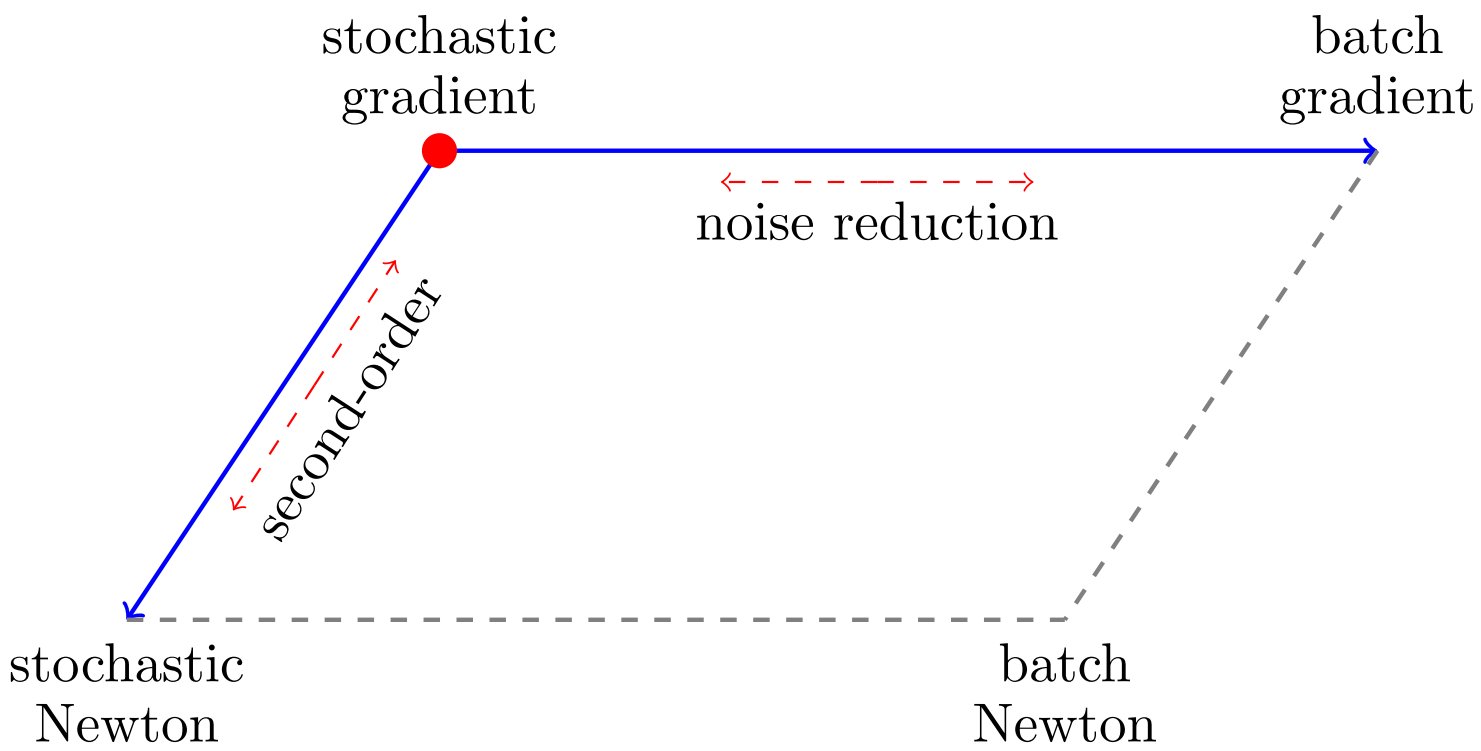
What can be improved?



What can be improved?



Two-dimensional schematic of methods



Nonconvex objectives

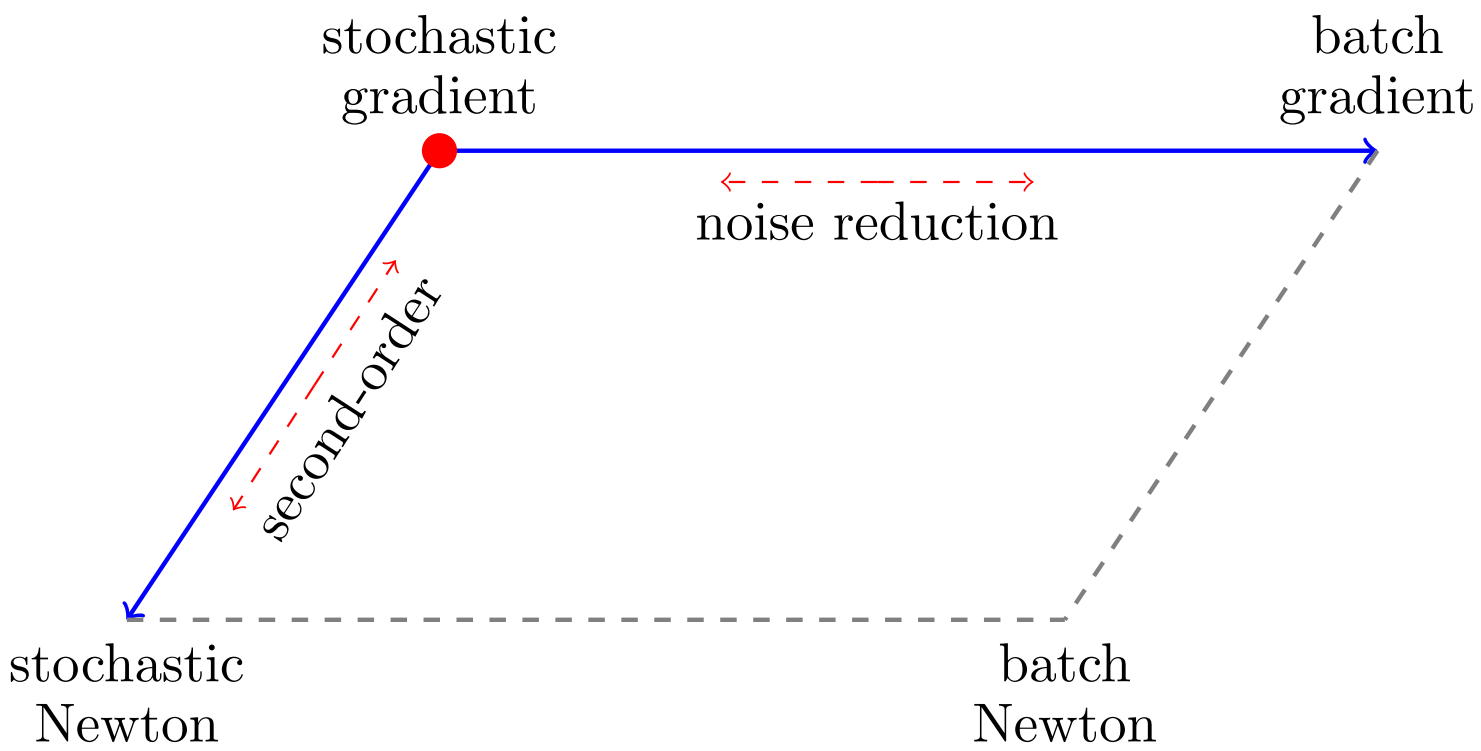
Despite loss of convergence rate, motivation for nonconvex problems as well:

- Convex results describe behavior near strong local minimizer
- Batch gradient methods are unlikely to get trapped near saddle points
- Second-order information can
  - avoid negative effects of nonlinearity and ill-conditioning
  - *require* mini-batching (noise reduction) to be efficient

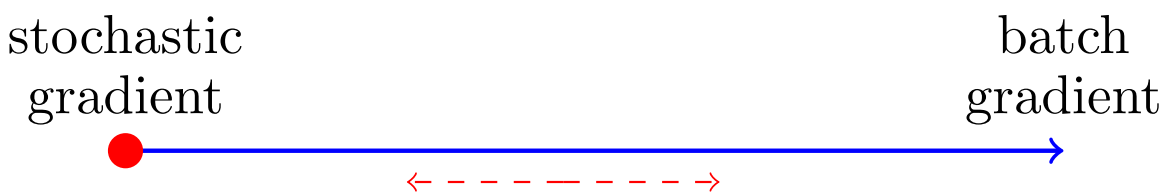
Conclusion: explore entire plane, not just one axis

Outline

Two-dimensional schematic of methods



2D schematic: Noise reduction methods



noise reduction

- dynamic sampling
- gradient aggregation
- iterate averaging

Ideal: Linear convergence of a batch gradient method

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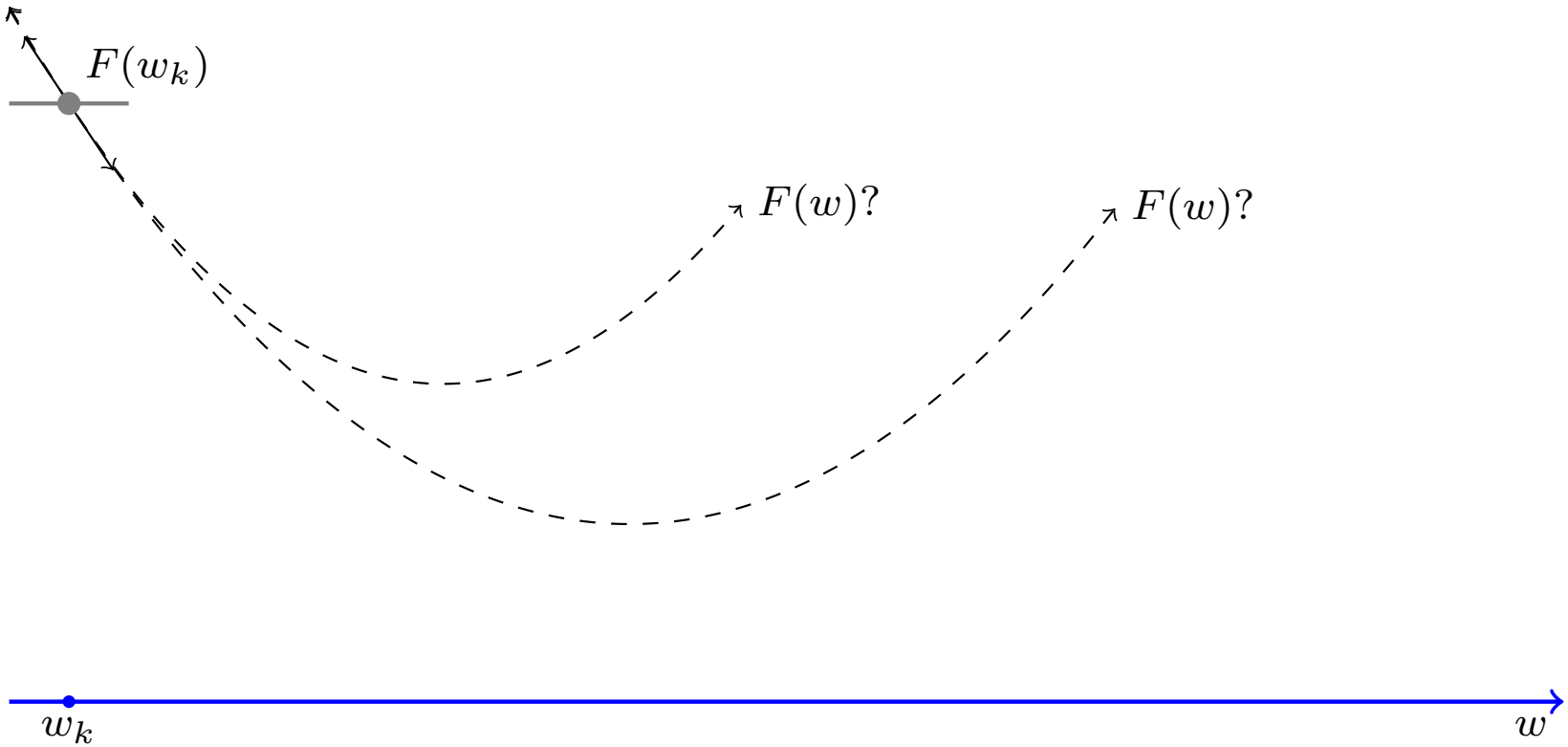
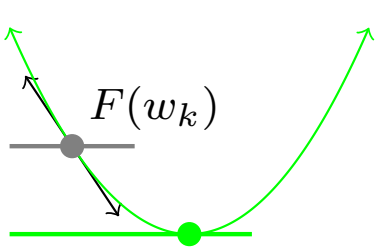
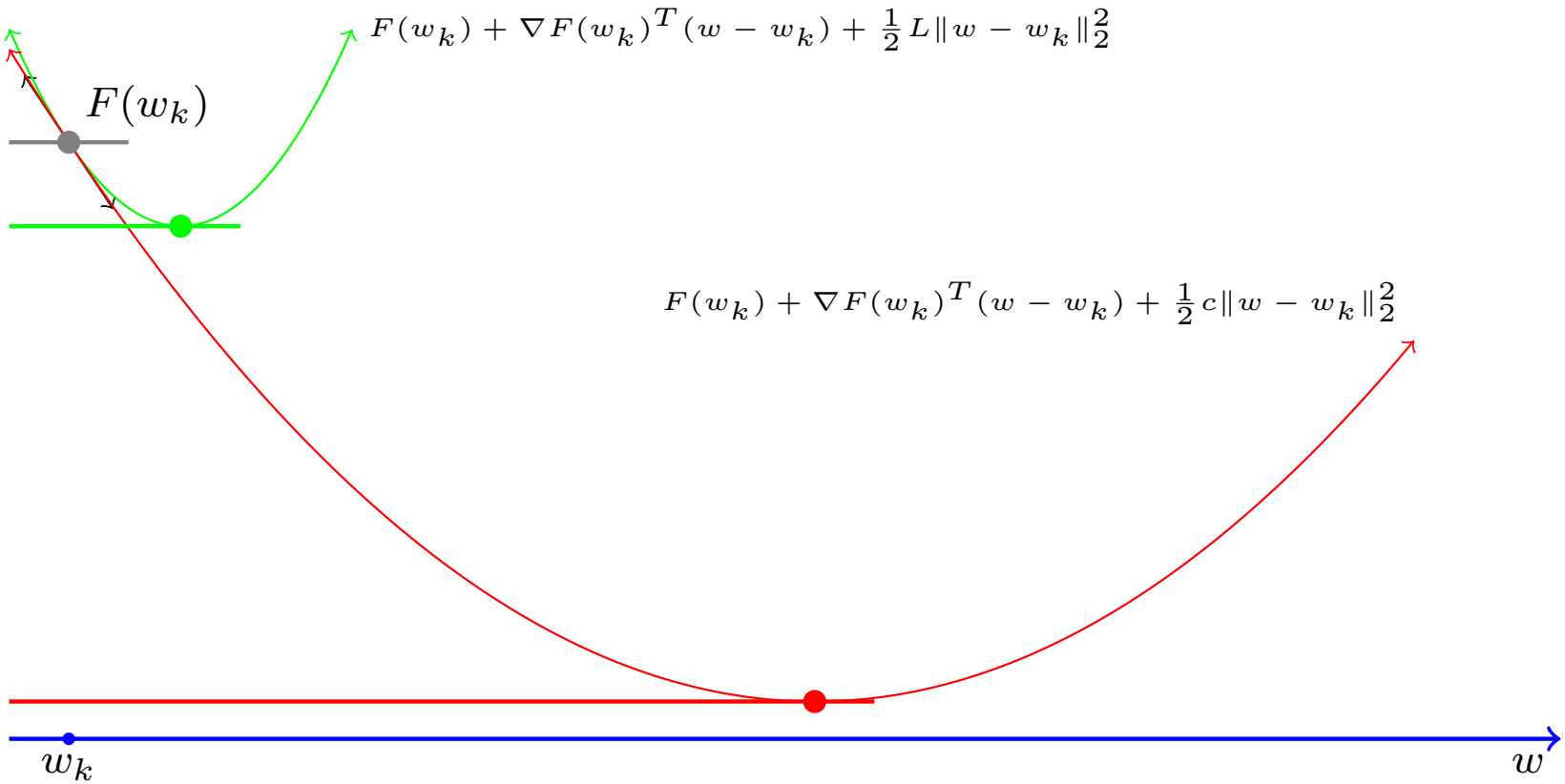


Ideal: Linear convergence of a batch gradient method



$$F(w_k) + \nabla F(w_k)^T (w - w_k) + \tfrac{1}{2} L \| w - w_k \|_2^2$$

Ideal: Linear convergence of a batch gradient method



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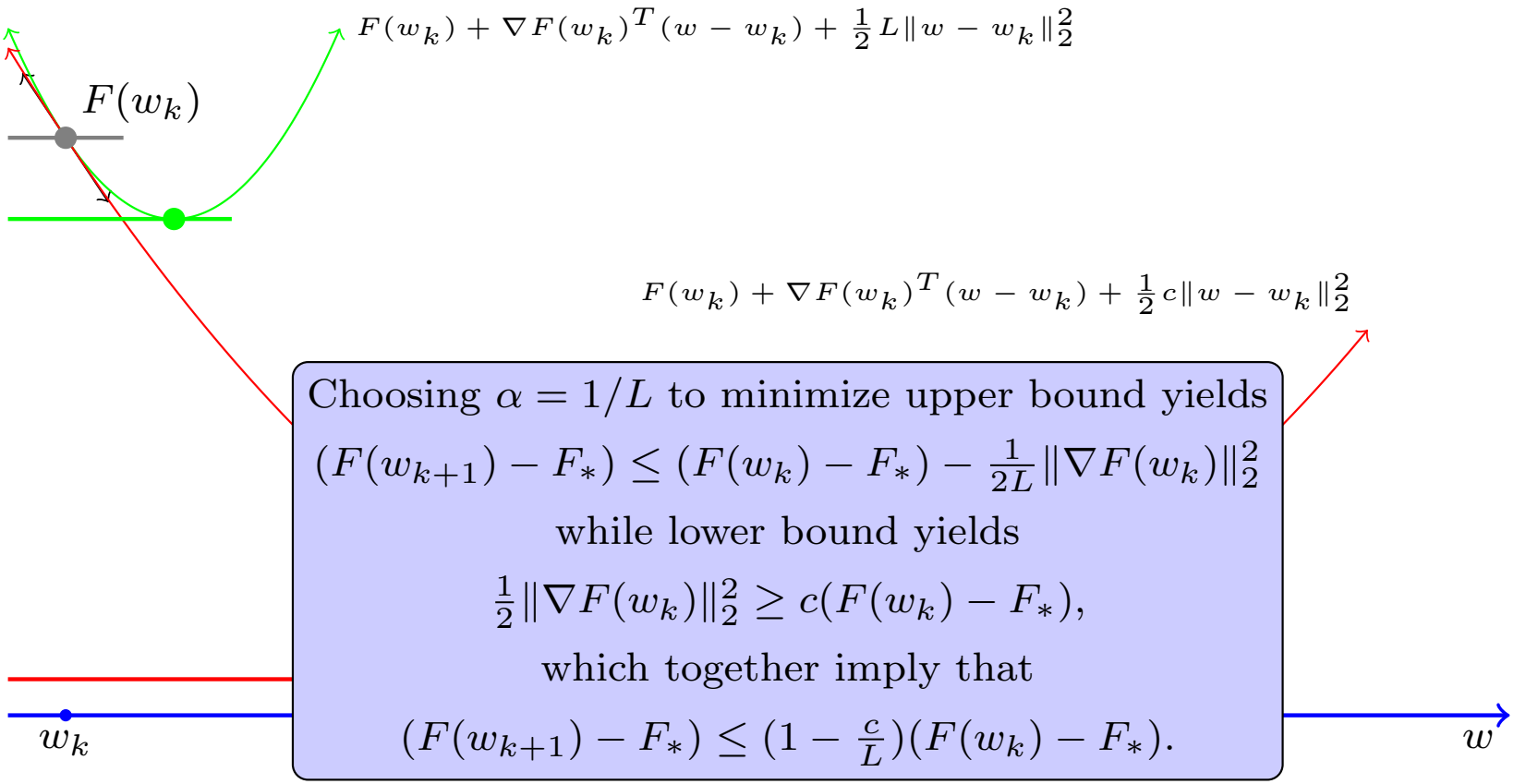

Choosing $\alpha = 1/L$ to minimize upper bound yields

$$(F(w_{k+1}) - F_*) \leq (F(w_k) - F_*) - \frac{1}{2L}\|\nabla F(w_k)\|_2^2$$

while lower bound yields

$$\frac{1}{2}\|\nabla F(w_k)\|_2^2 \geq c(F(w_k) - F_*),$$

which together imply that

$$(F(w_{k+1}) - F_*) \leq (1 - \tfrac{c}{L})(F(w_k) - F_*).$$

Illustration

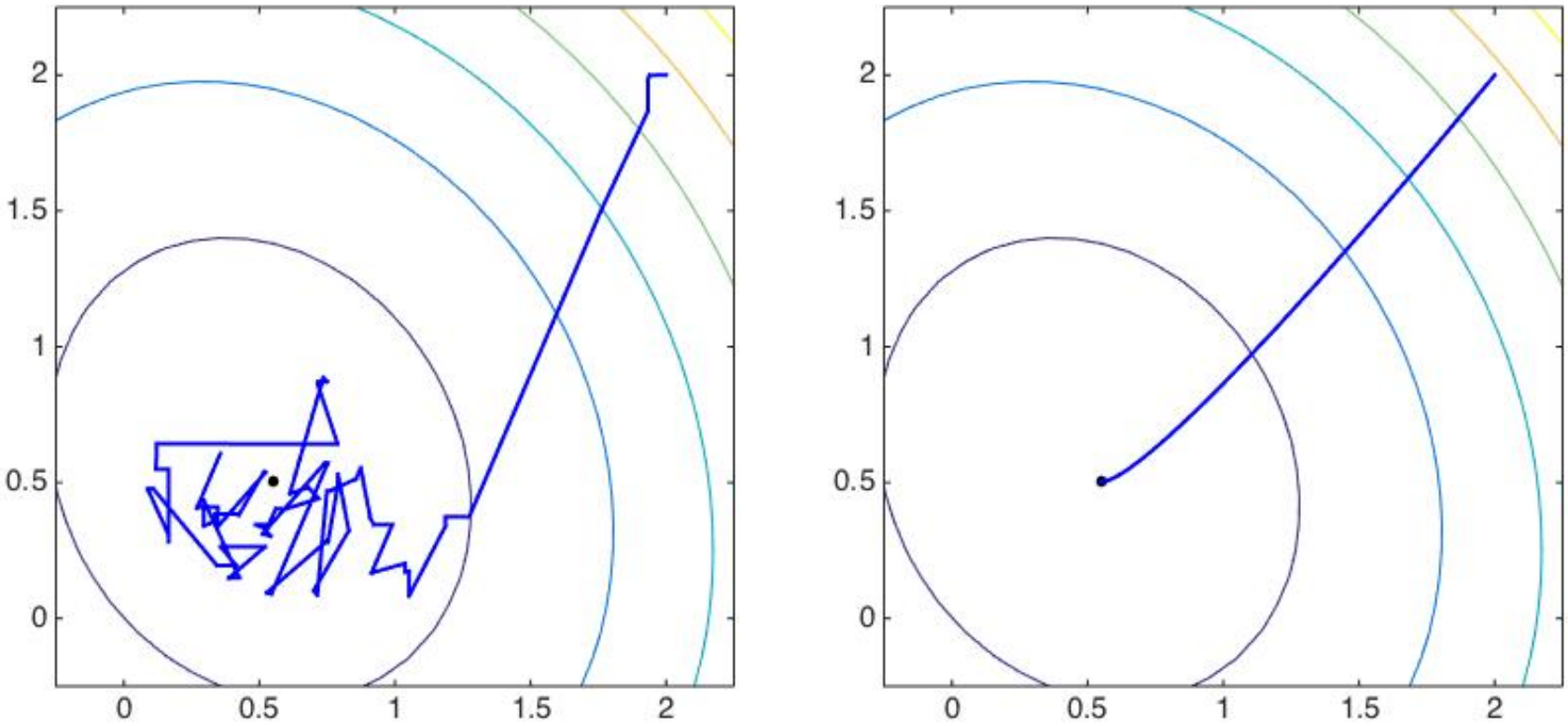

Figure: SG run with a fixed stepsize (left) vs. batch gradient with fixed stepsize (right)

Idea #1: Dynamic sampling

We have seen

- fast initial improvement by SG
- long-term linear rate achieved by batch gradient

$\Longrightarrow$ accumulate increasingly accurate gradient information during optimization.

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We have seen

- fast initial improvement by SG
- long-term linear rate achieved by batch gradient

$\Longrightarrow$ accumulate increasingly accurate gradient information during optimization.

But at what rate?

- too slow: won't achieve linear convergence
- too fast: loss of optimal work complexity

Geometric decrease

Correct balance achieved by decreasing noise at a geometric rate.

Theorem 3

Suppose Assumption $\langle L/c \rangle$ *holds and that*

$$\mathbb{V}_{\xi_k}[g(w_k, \xi_k)] \leq M\zeta^{k-1} \quad \textit{for some} \quad M \geq 0 \quad \textit{and} \quad \zeta \in (0, 1).$$

Then, the SG method with a fixed stepsize $\alpha = 1/L$ *yields*

$$\mathbb{E}[F(w_k) - F_*] \leq \omega\rho^{k-1},$$

where

$$\omega := \max\left\{\frac{M}{c}, F(w_1) - F_*\right\}$$

$$\textit{and} \quad \rho := \max\left\{1 - \frac{c}{2L}, \zeta\right\} < 1.$$

Effectively ties rate of noise reduction with convergence rate of optimization.

Geometric decrease

Proof.

The now familiar inequality

$$\mathbb{E}_{\xi_k}[F(w_{k+1})] - F(w_k) \leq -\alpha\|\nabla F(w_k)\|_2^2 + \tfrac{1}{2}\alpha^2 L\mathbb{E}_{\xi_k}[\|g(w_k,\xi_k)\|_2^2],$$

strong convexity, and the stepsize choice lead to

$$\mathbb{E}[F(w_{k+1}) - F_*] \leq \left(1 - \frac{c}{L}\right)\mathbb{E}[F(w_k) - F_*] + \frac{M}{2L}\zeta^{k-1}.$$

- Exactly as for batch gradient (in expectation) except for the last term.
- An inductive argument completes the proof.

Practical geometric decrease (unlimited samples)

How can geometric decrease of the variance be achieved in practice?

$$g_k := \frac{1}{|\mathcal{S}_k|} \sum_{i \in \mathcal{S}_k} \nabla f(w_k; \xi_{k,i}) \quad \text{with} \quad |\mathcal{S}_k| = \lceil \tau^{k-1} \rceil \quad \text{for} \quad \tau > 1,$$

since, for all $i \in \mathcal{S}_k$,

$$\mathbb{V}_{\xi_k}[g_k] \leq \frac{\mathbb{V}_{\xi_k}[\nabla f(w_k; \xi_{k,i})]}{|\mathcal{S}_k|} \leq M(\lceil \tau \rceil)^{k-1}.$$

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$$\mathbb{V}_{\xi_k}[g_k] \leq \frac{\mathbb{V}_{\xi_k}[\nabla f(w_k; \xi_{k,i})]}{|\mathcal{S}_k|} \leq M(\lceil \tau \rceil)^{k-1}.$$

But is it too fast? What about work complexity?

$$\text{same as SG as long as} \quad \tau \in \left(1, (1 - \frac{c}{2L})^{-1}\right].$$

Illustration

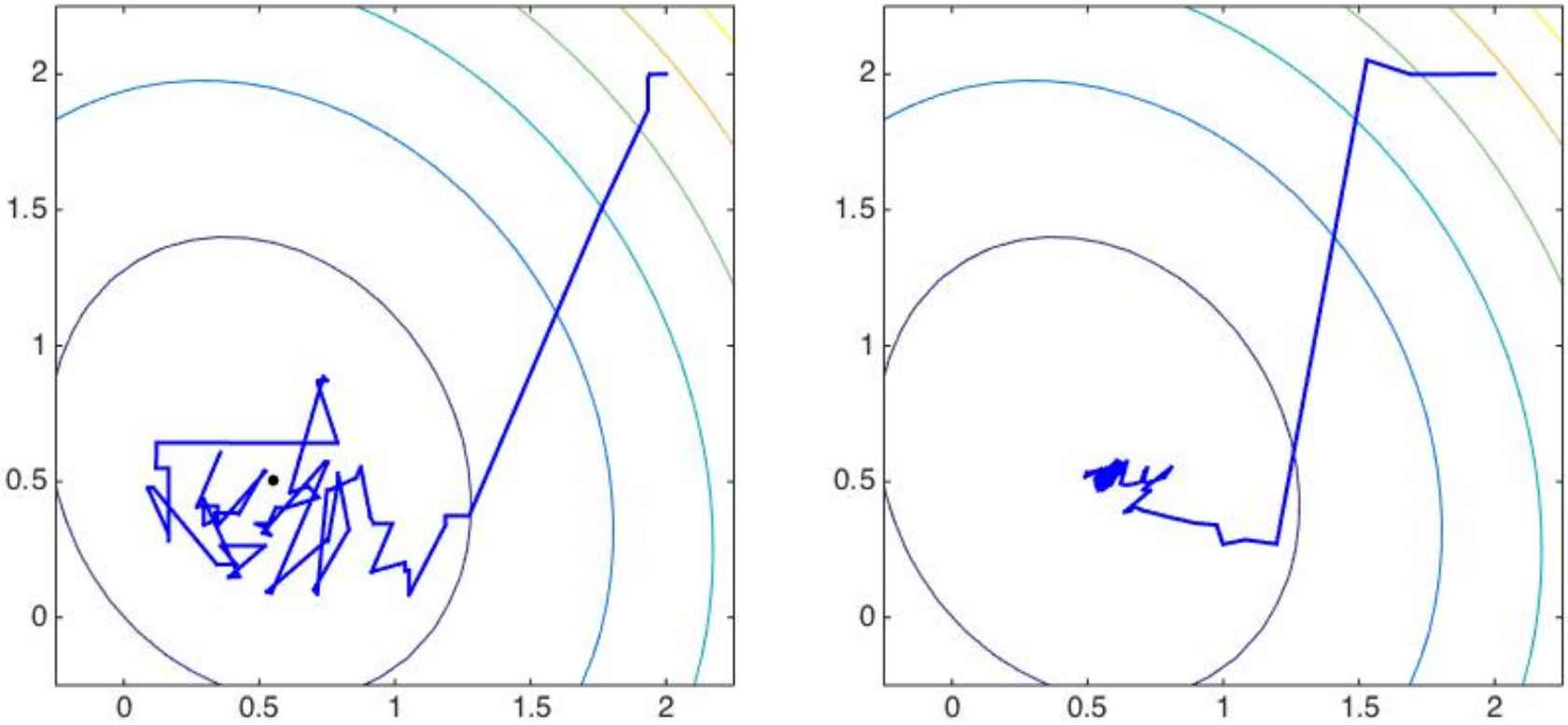


Figure: SG run with a fixed stepsize (left) vs. dynamic SG with fixed stepsize (right)

Additional considerations

In practice, choosing τ is a challenge.

- What about an adaptive technique?
- Guarantee descent in expectation
- Methods exist, but need geometric sample size increase as backup

Idea #2: Gradient aggregation

"I'm minimizing a finite sum and am willing to store previous gradient(s)."

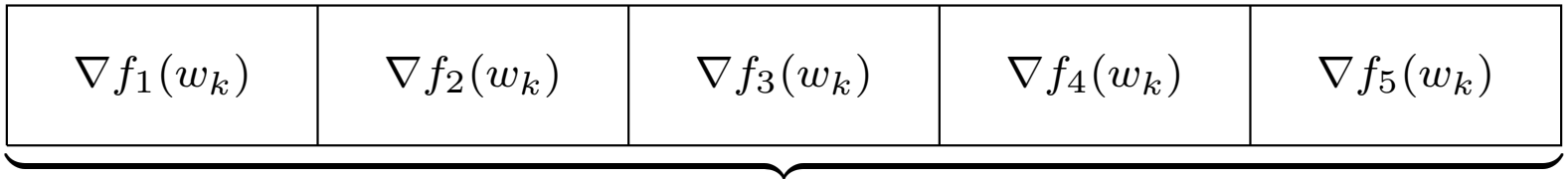
$$F(w) = R_n(w) = \frac{1}{n}\sum_{i=1}^{n} f_i(w).$$

Idea: reuse and/or revise previous gradient information in storage.

- SVRG: store full gradient, correct sequence of steps based on perceived bias
- SAGA: store *elements* of full gradient, revise as optimization proceeds

Stochastic variance reduced gradient (SVRG) method

At $w_k =: w_{k,1}$, compute a batch gradient:



then step

$$w_{k,2} \leftarrow w_{k,1} - \alpha g_{k,1}$$

Stochastic variance reduced gradient (SVRG) method

Now, iteratively, choose an index *randomly* and correct bias:

$\nabla f_1(w_k)$	$\nabla f_2(w_k)$	$\nabla f_3(w_k)$	$\nabla f_4(w_{k,2})$	$\nabla f_5(w_k)$

$$g_{k,2} \leftarrow \nabla F(w_k) - \nabla f_4(w_k) + \nabla f_4(w_{k,2})$$

then step

$$w_{k,3} \leftarrow w_{k,2} - \alpha g_{k,2}$$

Stochastic variance reduced gradient (SVRG) method

Now, iteratively, choose an index *randomly* and correct bias:

$\nabla f_1(w_k)$	$\nabla f_2(w_{k,3})$	$\nabla f_3(w_k)$	$\nabla f_4(w_k)$	$\nabla f_5(w_k)$

$$g_{k,3} \leftarrow \nabla F(w_k) - \nabla f_2(w_k) + \nabla f_2(w_{k,3})$$

then step

$$w_{k,4} \leftarrow w_{k,3} - \alpha g_{k,3}$$

Stochastic variance reduced gradient (SVRG) method

Each $g_{k,j}$ is an unbiased estimate of $\nabla F(w_{k,j})$!

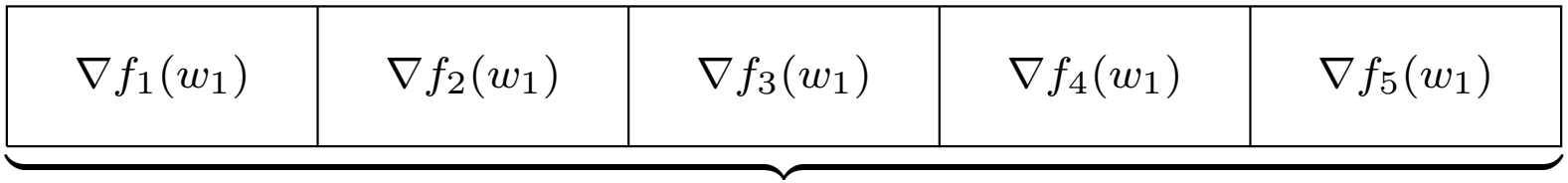
Algorithm SVRG

Choose an initial iterate $w_1 \in \mathbb{R}^d$, stepsize $\alpha > 0$, and positive integer m.
for $k = 1, 2, \ldots$ **do**
  Compute the batch gradient $\nabla F(w_k)$.
  Initialize $w_{k,1} \leftarrow w_k$.
  for $j = 1, \ldots, m$ **do**
    Chose i uniformly from $\{1, \ldots, n\}$.
    Set $g_{k,j} \leftarrow \nabla f_i(w_{k,j}) - (\nabla f_i(w_k) - \nabla F(w_k))$.
    Set $w_{k,j+1} \leftarrow w_{k,j} - \alpha g_{k,j}$.
  end for
  Option (a): Set $w_{k+1} = \tilde{w}_{m+1}$
  Option (b): Set $w_{k+1} = \frac{1}{m} \sum_{j=1}^{m} \tilde{w}_{j+1}$
  Option (c): Choose j uniformly from $\{1, \ldots, m\}$ and set $w_{k+1} = \tilde{w}_{j+1}$.
end for

Under Assumption $\langle L/c \rangle$, options (b) and (c) linearly convergent for certain (α, m)

Stochastic average gradient (SAGA) method

At w_1, compute a batch gradient:



$$g_1 \leftarrow \nabla F(w_1)$$

then step

$$w_2 \leftarrow w_1 - \alpha g_1$$

Stochastic average gradient (SAGA) method

Now, iteratively, choose an index *randomly* and revise table entry:

$\nabla f_1(w_1)$	$\nabla f_2(w_1)$	$\nabla f_3(w_1)$	$\nabla f_4(w_2)$	$\nabla f_5(w_1)$

$$g_2 \leftarrow \text{new entry} - \text{old entry} + \text{average of entries (before replacement)}$$

then step

$$w_3 \leftarrow w_2 - \alpha g_2$$

Stochastic average gradient (SAGA) method

Now, iteratively, choose an index *randomly* and revise table entry:

$\nabla f_1(w_1)$	$\nabla f_2(w_3)$	$\nabla f_3(w_1)$	$\nabla f_4(w_2)$	$\nabla f_5(w_1)$

$$g_3 \leftarrow \text{new entry} - \text{old entry} + \text{average of entries (before replacement)}$$

then step

$$w_4 \leftarrow w_3 - \alpha g_3$$

Stochastic average gradient (SAGA) method

Each g_k is an unbiased estimate of $\nabla F(w_k)$!

Algorithm SAGA

Choose an initial iterate $w_1 \in \mathbb{R}^d$ and stepsize $\alpha > 0$.
for $i = 1, \ldots, n$ **do**
    Compute $\nabla f_i(w_1)$.
    Store $\nabla f_i(w_{[i]}) \leftarrow \nabla f_i(w_1)$.
end for
for $k = 1, 2, \ldots$ **do**
    Choose j uniformly in $\{1, \ldots, n\}$.
    Compute $\nabla f_j(w_k)$.
    Set $g_k \leftarrow \nabla f_j(w_k) - \nabla f_j(w_{[j]}) + \frac{1}{n} \sum_{i=1}^n \nabla f_i(w_{[i]})$.
    Store $\nabla f_j(w_{[j]}) \leftarrow \nabla f_j(w_k)$.
    Set $w_{k+1} \leftarrow w_k - \alpha g_k$.
end for

Under Assumption $\langle L/c \rangle$, linearly convergent for certain α

- storage of gradient vectors reasonable in some applications
- with access to feature vectors, need only store n scalars

Idea #3: Iterative averaging

Averages of SG iterates are less noisy:

$$w_{k+1} \leftarrow w_k - \alpha_k g(w_k, \xi_k)$$

$$\tilde{w}_{k+1} \leftarrow \frac{1}{k+1} \sum_{j=1}^{k+1} w_j \quad \text{(in practice: running average)}$$

Unfortunately, no better theoretically when $\alpha_k = \mathcal{O}(1/k)$, but

- long steps (say, $\alpha_k = \mathcal{O}(1/\sqrt{k})$) *and* averaging
- lead to a better sublinear rate (like a second-order method?)

See also

- mirror descent
- primal-dual averaging

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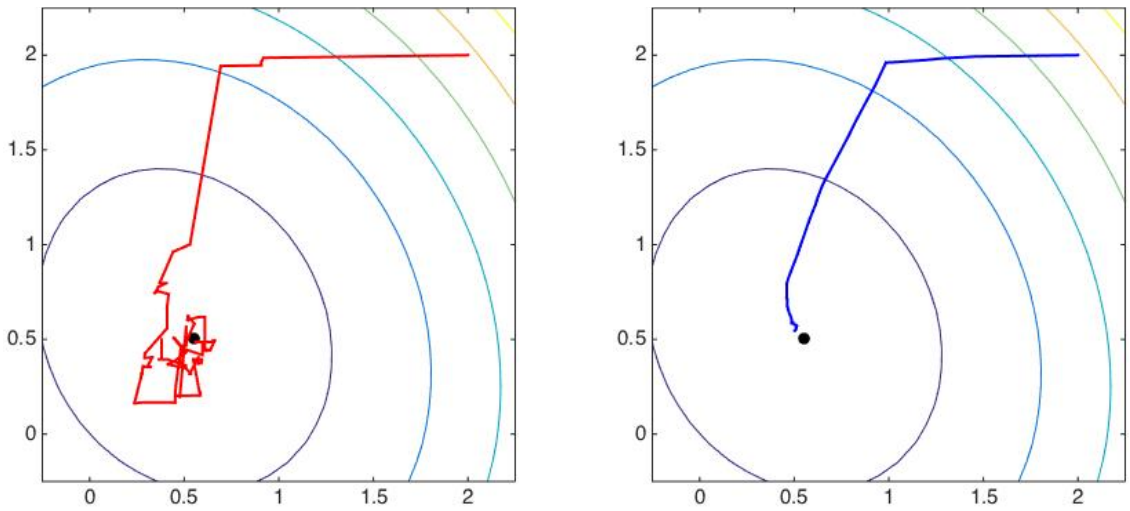
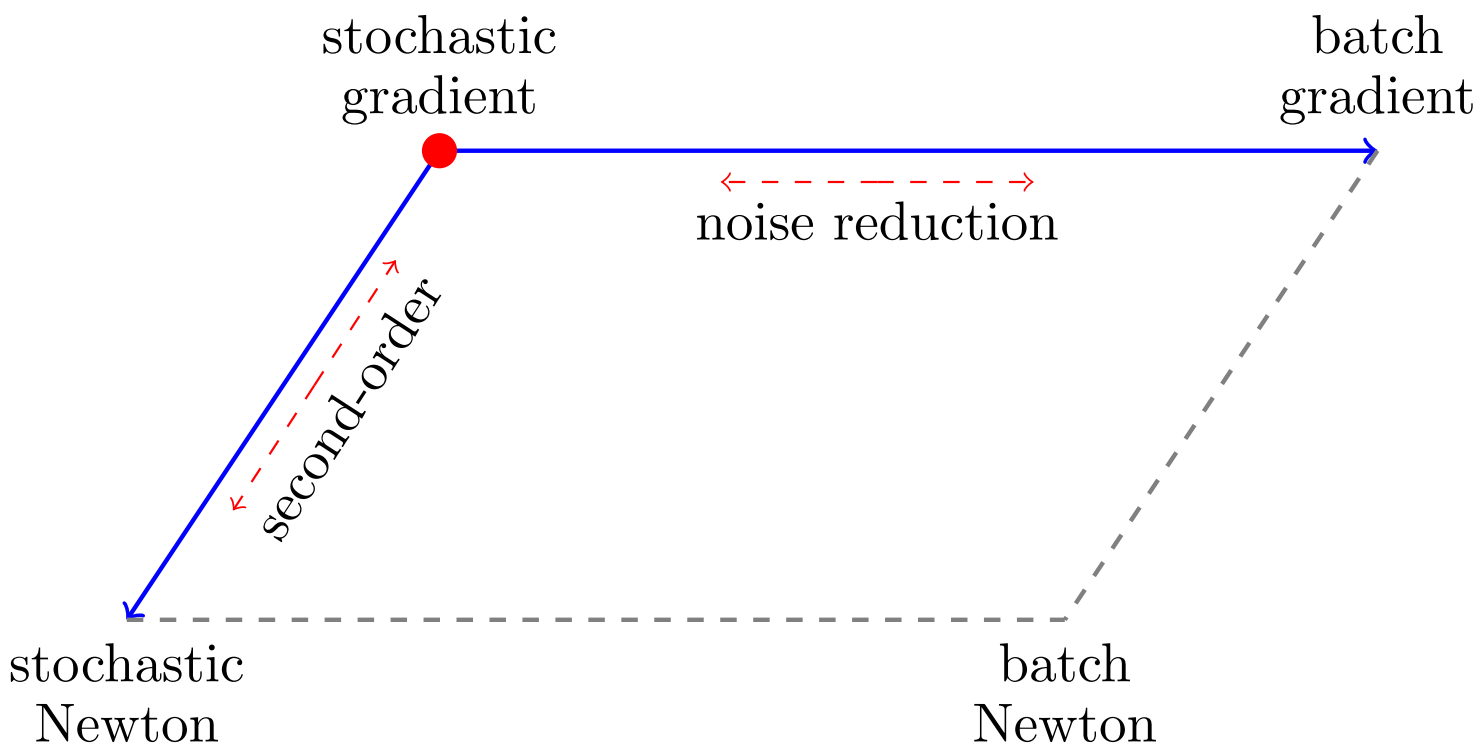


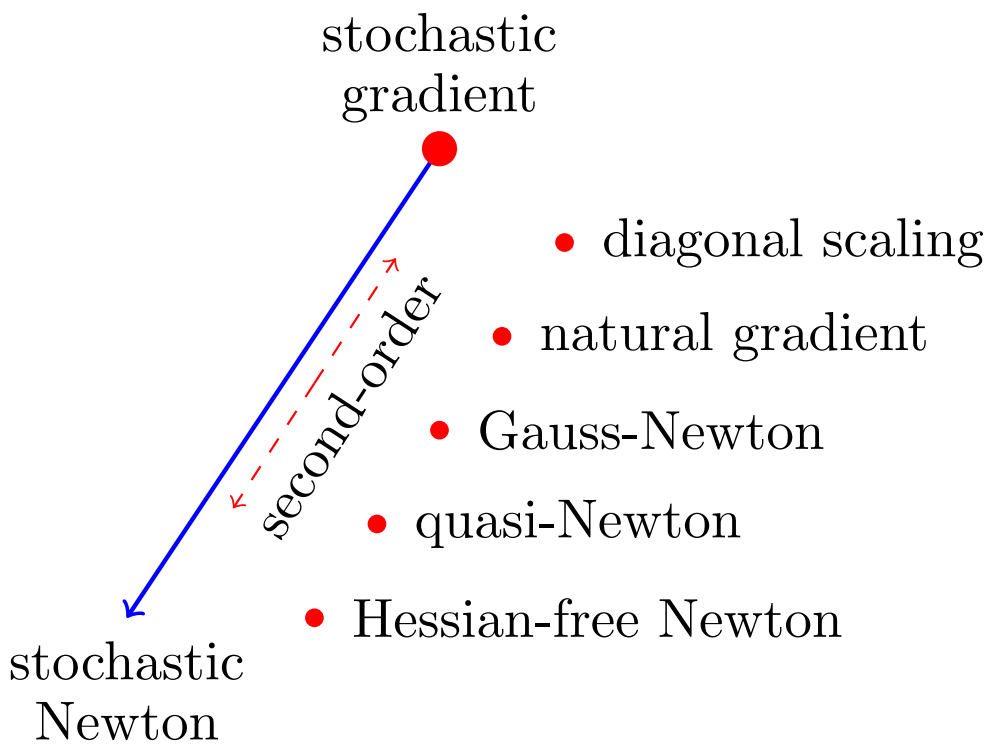
Figure: SG run with $\mathcal{O}(1/\sqrt{k})$ stepsizes (left) vs. sequence of averages (right)

Outline

Two-dimensional schematic of methods



2D schematic: Second-order methods



Ideal: Scale invariance

Neither SG nor batch gradient are invariant to linear transformations!

$$\min_{w\in\mathbb{R}^d} F(w) \qquad \Longrightarrow \qquad w_{k+1} \leftarrow w_k - \alpha_k \nabla F(w_k)$$

$$\min_{\tilde{w}\in\mathbb{R}^d} F(B\tilde{w}) \qquad \Longrightarrow \qquad \tilde{w}_{k+1} \leftarrow \tilde{w}_k - \alpha_k B \nabla F(B\tilde{w}_k) \quad \text{(for given } B \succ 0\text{)}$$

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$$\min_{\tilde{w}\in\mathbb{R}^d} F(B\tilde{w}) \qquad \Longrightarrow \qquad \tilde{w}_{k+1} \leftarrow \tilde{w}_k - \alpha_k B \nabla F(B\tilde{w}_k) \quad \text{(for given } B \succ 0)$$

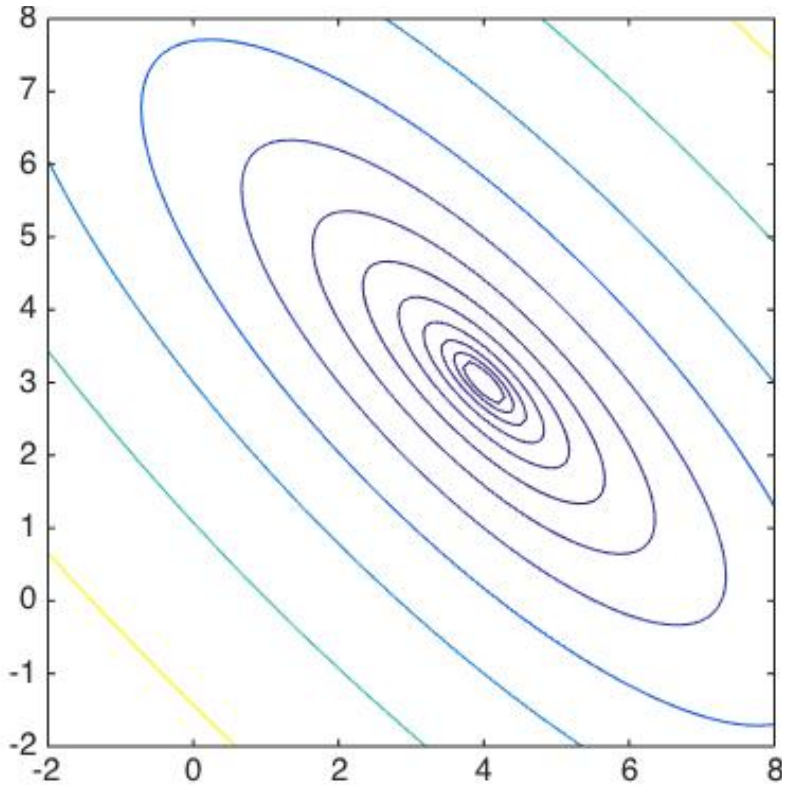
Scaling latter by B and defining $\{w_k\} = \{B\tilde{w}_k\}$ yields

$$w_{k+1} \leftarrow w_k - \alpha_k B^2 \nabla F(w_k)$$

- Algorithm is clearly affected by choice of B
- Surely, some choices may be better than others (in general?)

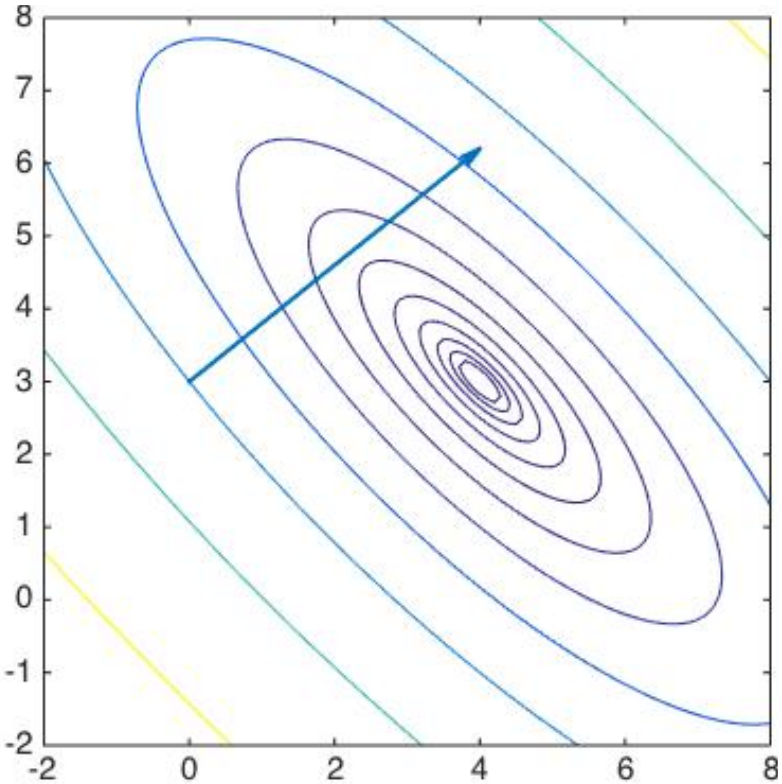
Newton scaling

Consider the function below and suppose that $w_k = (0, 3)$:



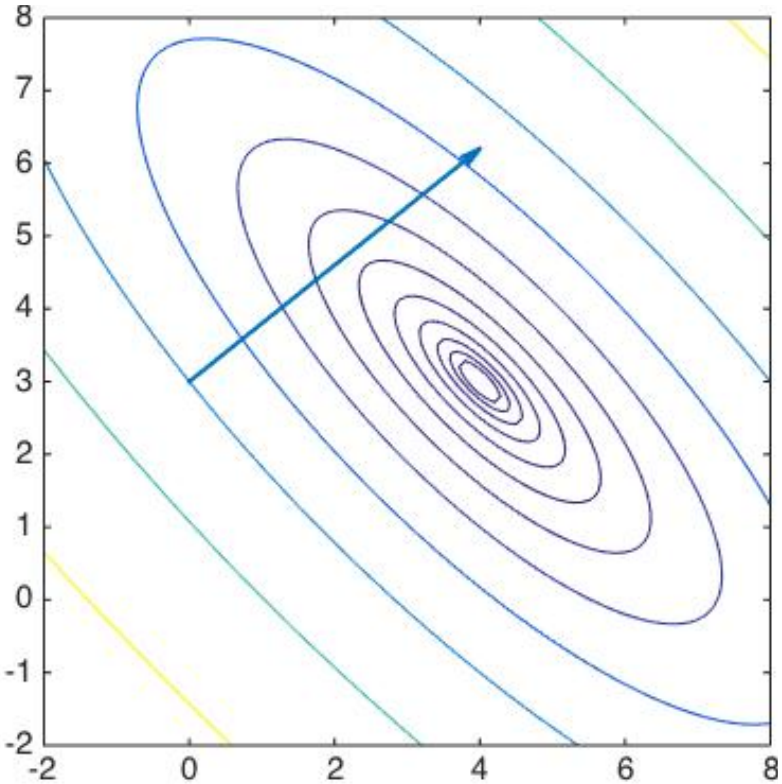
Newton scaling

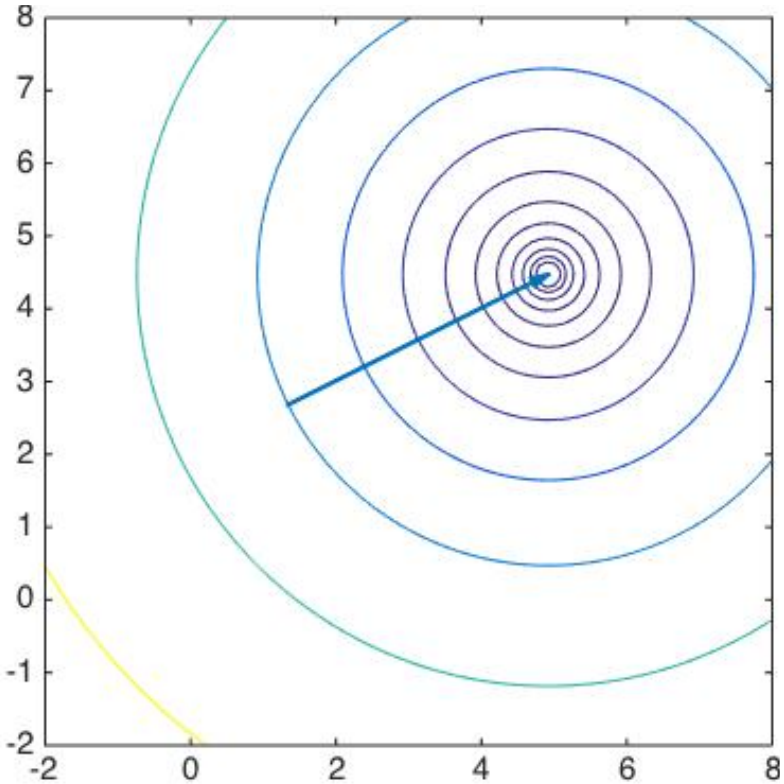
Batch gradient step $-\alpha_k \nabla F(w_k)$ ignores curvature of the function:



Newton scaling

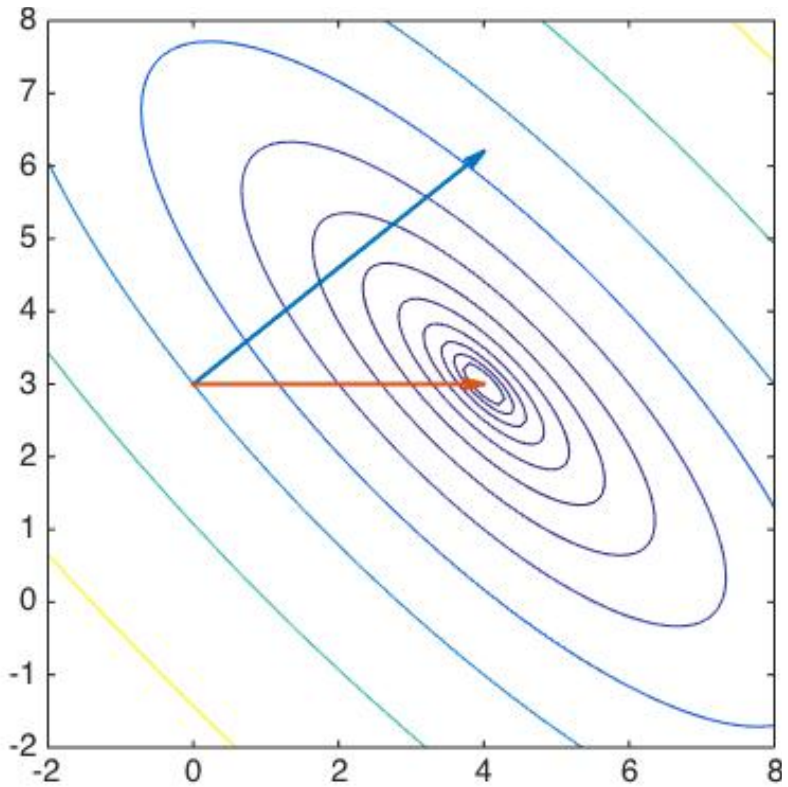
Newton scaling ($B = (\nabla F(w_k))^{-1/2}$): gradient step moves to the minimizer:

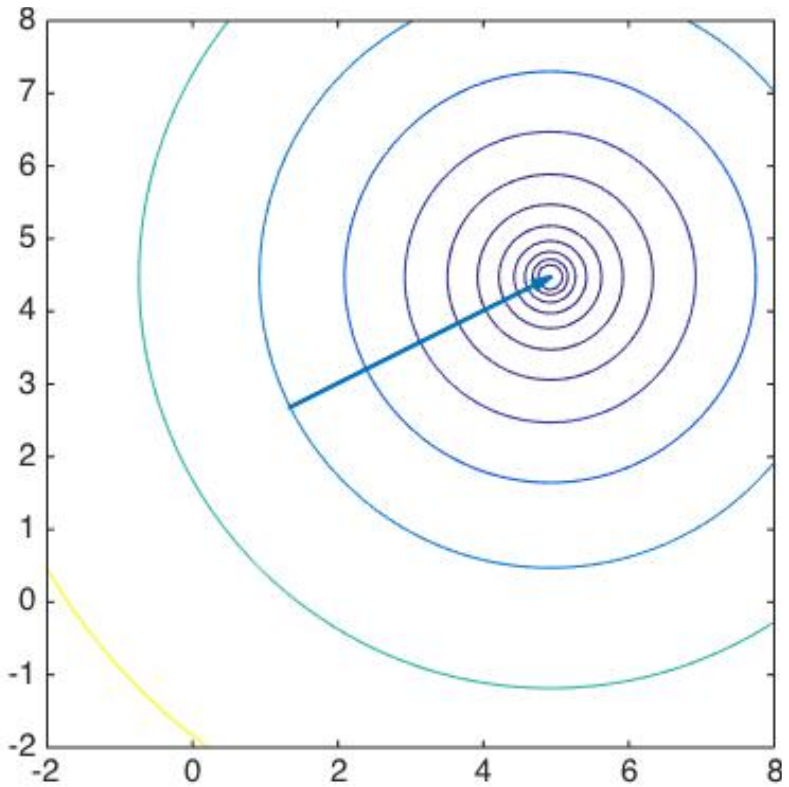




Newton scaling

. . . corresponds to minimizing a quadratic model of F in the original space:





$$w_{k+1} \leftarrow w_k + \alpha_k s_k \quad \text{where} \quad \nabla^2 F(w_k) s_k = -\nabla F(w_k)$$

Deterministic case

What is known about Newton's method for deterministic optimization?

- local rescaling based on inverse Hessian information
- locally quadratically convergent near a strong minimizer
- global convergence rate better than gradient method (*when regularized*)

Deterministic case to stochastic case

What is known about Newton's method for deterministic optimization?

- local rescaling based on inverse Hessian information
- locally quadratically convergent near a strong minimizer
- global convergence rate better than gradient method (*when regularized*)

However, it is way too expensive in our case.

- But all is not lost: scaling is viable.
- Wide variety of scaling techniques improve performance.
- Our convergence theory for SG still holds with B-scaling.
- . . . could hope to remove condition number (L/c) from convergence rate!
- Added costs can be minimial when coupled with noise reduction.

Idea #1: Inexact Hessian-free Newton

Compute Newton-like step

$$\nabla^2 f_{\mathcal{S}_k^H}(w_k) s_k = -\nabla f_{\mathcal{S}_k^g}(w_k)$$

- mini-batch size for Hessian =: $|\mathcal{S}_k^H| < |\mathcal{S}_k^g|$:= mini-batch size for gradient
- cost for mini-batch gradient: g_{cost}
- use CG and terminate early: max_{cg} iterations
- in CG, cost for each Hessian-vector product: $factor \times g_{cost}$
- choose $max_{cg} \times factor \approx$ small constant so total per-iteration cost:

$$max_{cg} \times factor \times g_{cost} = \mathcal{O}(g_{cost})$$

- convergence guarantees for $|\mathcal{S}_k^H| = |\mathcal{S}_k^g| = n$ are well-known

Idea #2: (Generalized) Gauss-Newton

Classical approach for nonlinear least squares, linearize inside of loss/cost:

$$\begin{aligned} f(w;\xi) &= \tfrac{1}{2}\|h(x_\xi;w) - y_\xi\|_2^2 \\ &\approx \tfrac{1}{2}\|h(x_\xi;w_k) + J_h(w_k;\xi)(w-w_k) - y_\xi\|_2^2 \end{aligned}$$

Leads to Gauss-Newton approximation for second-order terms:

$$G_{\mathcal{S}_k^H}(w_k;\xi_k^H) = \frac{1}{|\mathcal{S}_k^H|} J_h(w_k;\xi_{k,i})^T J_h(w_k;\xi_{k,i})$$

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$$\begin{aligned} f(w;\xi) &= \tfrac{1}{2}\|h(x_\xi;w) - y_\xi\|_2^2 \\ &\approx \tfrac{1}{2}\|h(x_\xi;w_k) + J_h(w_k;\xi)(w-w_k) - y_\xi\|_2^2 \end{aligned}$$

Leads to Gauss-Newton approximation for second-order terms:

$$G_{\mathcal{S}_k^H}(w_k;\xi_k^H) = \frac{1}{|\mathcal{S}_k^H|} J_h(w_k;\xi_{k,i})^T J_h(w_k;\xi_{k,i})$$

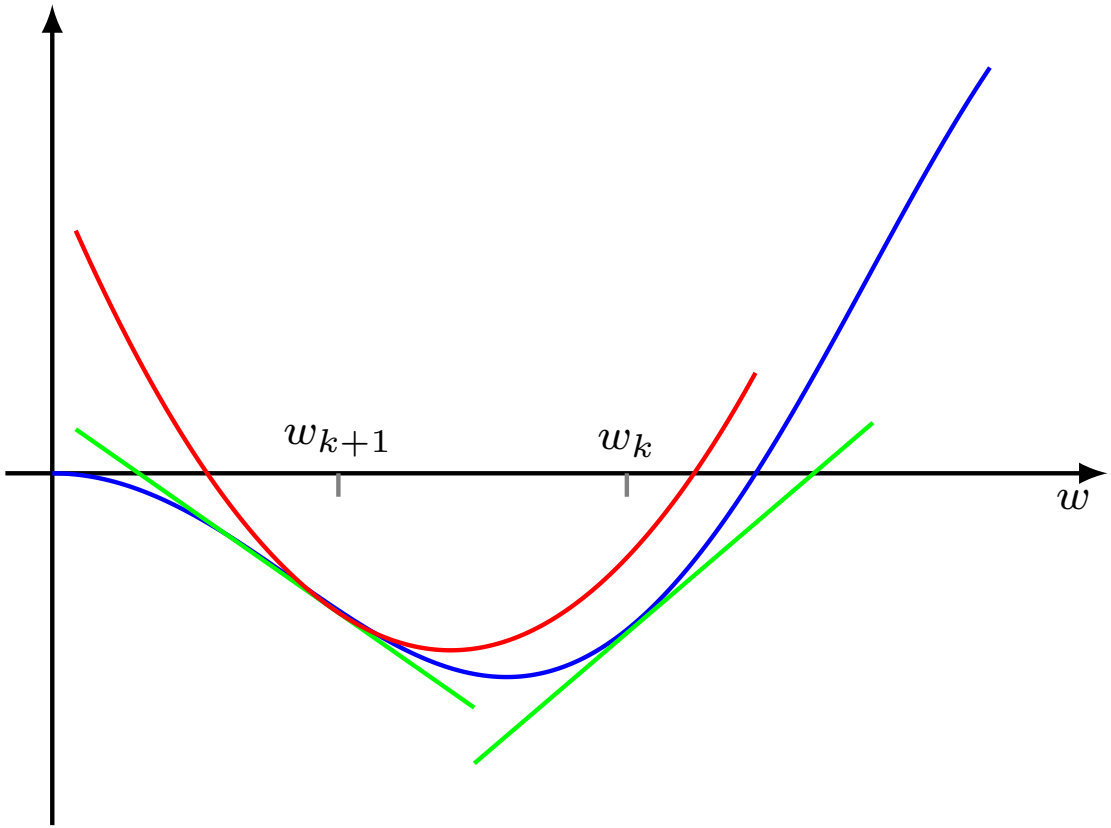
Can be generalized for other (convex) losses:

$$\widetilde{G}_{\mathcal{S}_k^H}(w_k;\xi_k^H) = \frac{1}{|\mathcal{S}_k^H|} J_h(w_k;\xi_{k,i})^T \underbrace{H_\ell(w_k;\xi_{k,i})}_{=\frac{\partial^2 \ell}{\partial h^2}} J_h(w_k;\xi_{k,i})$$

- costs similar as for inexact Newton
- . . . but scaling matrices are always positive (semi)definite
- see also *natural gradient*, invariant to more than just linear transformations

Idea #3: (Limited memory) quasi-Newton

Only *approximate* second-order information with gradient displacements:



Secant equation $H_k v_k = s_k$ to match gradient of F at w_k, where

$$s_k := w_{k+1} - w_k \quad \text{and} \quad v_k := \nabla F(w_{k+1}) - \nabla F(w_k)$$

Deterministic case

Standard update for inverse Hessian ($w_{k+1} \leftarrow w_k - \alpha_k H_k g_k$) is BFGS:

$$H_{k+1} \leftarrow \left(I - \frac{v_k s_k^T}{s_k^T v_k}\right)^T H_k \left(I - \frac{v_k s_k^T}{s_k^T v_k}\right) + \frac{s_k s_k^T}{s_k^T v_k}$$

What is known about quasi-Newton methods for deterministic optimization?

- local rescaling based on iterate/gradient displacements
- strongly convex function $\implies$ positive definite (p.d.) matrices
- only first-order derivatives, no linear system solves
- locally superlinearly convergent near a strong minimizer

Deterministic case to stochastic case

Standard update for inverse Hessian ($w_{k+1} \leftarrow w_k - \alpha_k H_k g_k$) is BFGS:

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What is known about quasi-Newton methods for deterministic optimization?

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Extended to stochastic case? How?

- Noisy gradient estimates $\implies$ challenge to maintain p.d.
- Correlation between gradient and Hessian estimates
- Overwriting updates $\implies$ poor scaling that plagues!

Proposed methods

- gradient displacements using same sample:

$$v_k := \nabla f_{\mathcal{S}_k}(w_{k+1}) - \nabla f_{\mathcal{S}_k}(w_k)$$

  (requires two stochastic gradients per iteration)
- gradient displacement replaced by action on subsampled Hessian:

$$v_k := \nabla^2 f_{\mathcal{S}_k^H}(w_k)(w_{k+1} - w_k)$$

- decouple iteration and Hessian update to amortize added cost
- limited memory approximations (e.g., L-BFGS) with per-iteration cost $4md$

Idea #4: Diagonal scaling

Restrict added costs through only diagonal scaling:

$$w_{k+1} \leftarrow w_k - \alpha_k D_k g_k$$

Ideas:

- $D_k^{-1} \approx$ diag(Hessian (approximation))
- $D_k^{-1} \approx$ diag(Gauss-Newton approximation)
- $D_k^{-1} \approx$ running average/sum of gradient components

Last approach can be motivated by minimizing regret.

Outline

Plenty of ideas not covered here!

- gradient methods with momentum
- gradient methods with acceleration
- coordinate descent/ascent in the primal/dual
- proximal gradient/Newton for regularized problems
- alternating direction methods
- expectation-maximization
- ...