Beyond stochastic gradient descent for large-scale machine learning

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Joint work with Eric Moulines - September 2014

Context

Machine learning for "big data"

- **Large-scale machine learning**: **large p, large n**
  - p : dimension of each observation (input)
  - n : number of observations
- **Examples**: computer vision, bioinformatics, advertising

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- **Examples**: computer vision, bioinformatics, advertising
- **Ideal running-time complexity**: $O(pn)$
- **Going back to simple methods**
  - Stochastic gradient methods (Robbins and Monro, 1951)
  - Mixing statistics and optimization

Supervised machine learning

- **Data**: n observations $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$, $i = 1, \dots, n$, **i.i.d.**
- Prediction as a linear function $\langle \theta, \Phi(x) \rangle$ of features $\Phi(x) \in \mathbb{R}^p$
- **(regularized) empirical risk minimization**: find $\hat{\theta}$ solution of

$$\min_{\theta \in \mathbb{R}^p} \quad \frac{1}{n} \sum_{i=1}^{n} \ell\big(y_i, \langle \theta, \Phi(x_i) \rangle\big) \quad + \quad \mu \Omega(\theta)$$

convex data fitting term + regularizer

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- Empirical risk: $\hat{f}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, \langle \theta, \Phi(x_i) \rangle)$ training cost
- Expected risk: $f(\theta) = \mathbb{E}_{(x,y)} \ell(y, \langle \theta, \Phi(x) \rangle)$ testing cost
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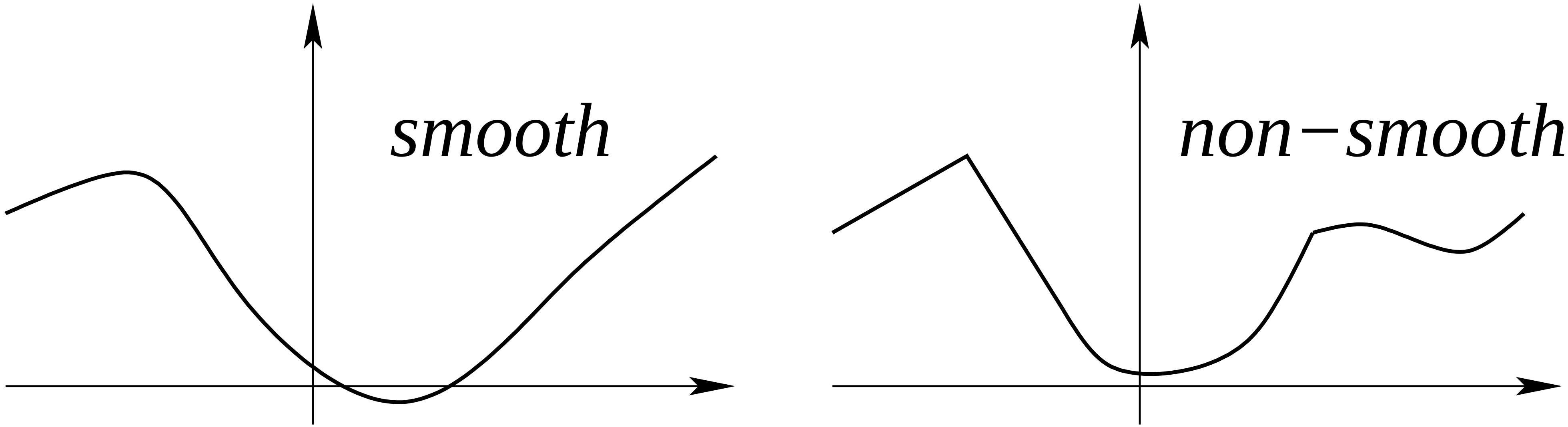
- **Two fundamental questions**: (1) computing $\hat{\theta}$ and (2) analyzing $\hat{\theta}$
  - **May be tackled simultaneously**

Smoothness and strong convexity

- A function $g : \mathbb{R}^p \to \mathbb{R}$ is L-smooth if and only if it is twice differentiable and

$$\forall \theta \in \mathbb{R}^p, \ g''(\theta) \preccurlyeq L \cdot \mathrm{Id}$$



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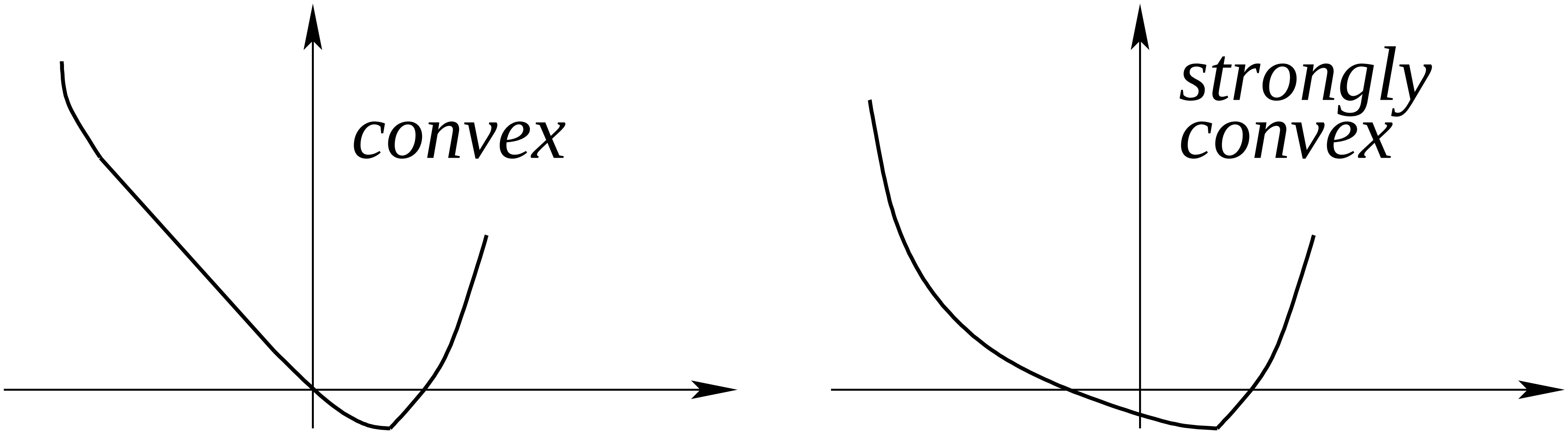
- **Machine learning**
  - with $g(\theta) = \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, \langle \theta, \Phi(x_i) \rangle)$
  - Hessian $\approx$ covariance matrix $\frac{1}{n}\sum_{i=1}^{n} \Phi(x_i) \otimes \Phi(x_i)$
  - Bounded data

Smoothness and strong convexity

- A twice differentiable function $g : \mathbb{R}^p \rightarrow \mathbb{R}$ is μ-strongly convex if and only if

$$\forall \theta \in \mathbb{R}^p, \; g''(\theta) \succcurlyeq \mu \cdot \mathrm{Id}$$



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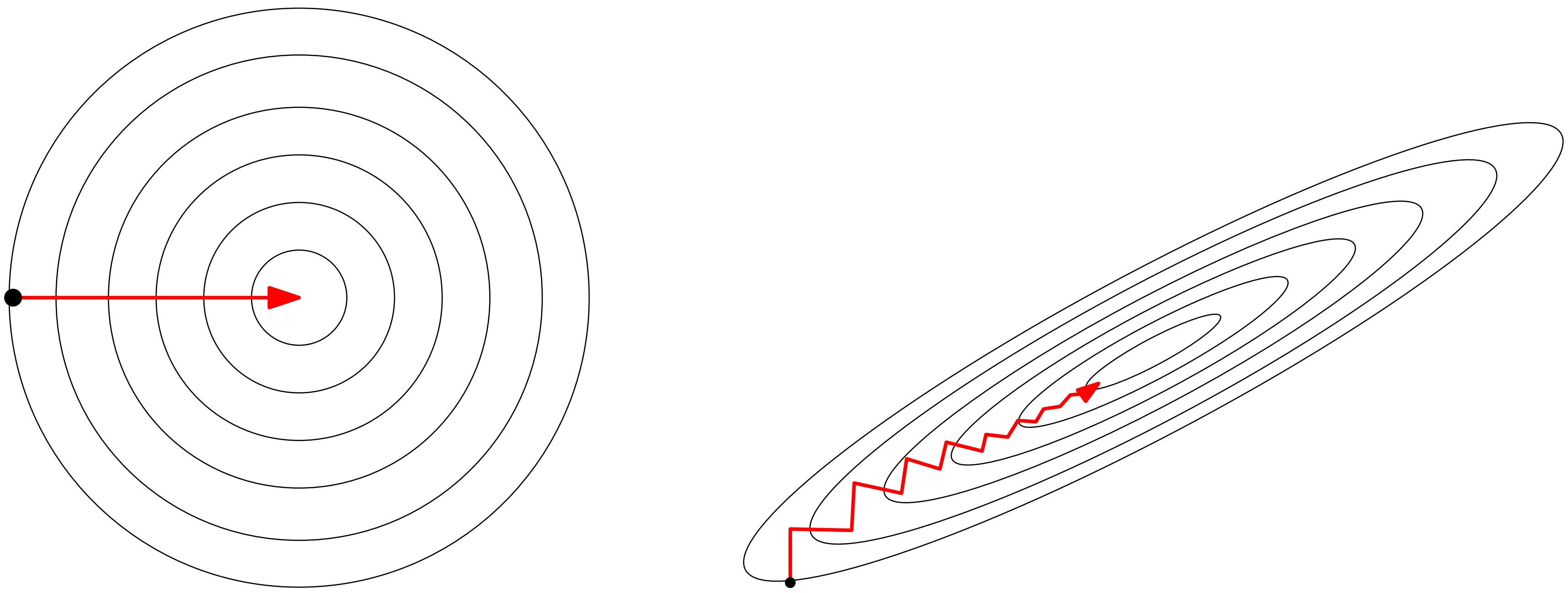
- **Adding regularization by $\frac{\mu}{2}\|\theta\|^2$**
  - creates additional bias unless μ is small

Iterative methods for minimizing smooth functions

- **Assumption**: g convex and smooth on $\mathbb{R}^p$

- **Gradient descent**: $\theta_t = \theta_{t-1} - \gamma_t \, g'(\theta_{t-1})$
  - $O(1/t)$ convergence rate for convex functions
  - $O(e^{-\rho t})$ convergence rate for strongly convex functions



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- **Key insights from Bottou and Bousquet (2008)**
  1. In machine learning, no need to optimize below statistical error
  2. In machine learning, cost functions are averages

$\Rightarrow$ **Stochastic approximation**

Stochastic approximation

- **Goal**: Minimizing a function f defined on $\mathbb{R}^p$
  - given only unbiased estimates $f'_n(\theta_n)$ of its gradients $f'(\theta_n)$ at certain points $\theta_n \in \mathbb{R}^p$

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- **Machine learning - statistics**
  - $f(\theta) = \mathbb{E} f_n(\theta) = \mathbb{E}\, \ell(y_n, \langle \theta, \Phi(x_n)\rangle) =$ **generalization error**
  - **Loss for a single pair of observations**: $f_n(\theta) = \ell(y_n, \langle \theta, \Phi(x_n)\rangle)$
  - Expected gradient:

$$f'(\theta) = \mathbb{E} f'_n(\theta) = \mathbb{E}\left\{\ell'(y_n, \langle \theta, \Phi(x_n)\rangle)\, \Phi(x_n)\right\}$$

- Beyond convex optimization: see, e.g., Benveniste et al. (2012)

Convex stochastic approximation

- **Key assumption**: smoothness and/or strong convexity
- **Key algorithm:** stochastic gradient descent (a.k.a. Robbins-Monro)

$$\boxed{\theta_n = \theta_{n-1} - \gamma_n f_n'(\theta_{n-1})}$$

  – Polyak-Ruppert averaging: $\bar{\theta}_n = \frac{1}{n+1}\sum_{k=0}^{n} \theta_k$

  – Which learning rate sequence γ_n? Classical setting: $\boxed{\gamma_n = Cn^{-\alpha}}$

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- **Running-time** $= O(np)$
  – Single pass through the data
  – One line of code among many

Convex stochastic approximation
Existing work

- **Known global minimax rates of convergence for non-smooth problems** (Nemirovsky and Yudin, 1983; Agarwal et al., 2012)
  - Strongly convex: $O((\mu n)^{-1})$
    Attained by averaged stochastic gradient descent with $\gamma_n \propto (\mu n)^{-1}$
  - Non-strongly convex: $O(n^{-1/2})$
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- **Asymptotic analysis of averaging** (Polyak and Juditsky, 1992; Ruppert, 1988)
  - All step sizes $\gamma_n = Cn^{-\alpha}$ with $\alpha \in (1/2, 1)$ lead to $O(n^{-1})$ for smooth strongly convex problems

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- **A single algorithm for smooth problems with convergence rate $O(1/n)$ in all situations?**

Least-mean-square algorithm

- **Least-squares**: $f(\theta) = \frac{1}{2}\mathbb{E}\big[(y_n - \langle \Phi(x_n), \theta \rangle)^2\big]$ with $\theta \in \mathbb{R}^p$
  - SGD $=$ least-mean-square algorithm (see, e.g., Macchi, 1995)
  - usually studied without averaging and decreasing step-sizes
  - with strong convexity assumption $\mathbb{E}\big[\Phi(x_n) \otimes \Phi(x_n)\big] = H \succcurlyeq \mu \cdot \mathrm{Id}$

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- **New analysis for averaging and constant step-size** $\gamma = 1/(4R^2)$
  - Assume $\|\Phi(x_n)\| \leqslant R$ and $|y_n - \langle \Phi(x_n), \theta_*\rangle| \leqslant \sigma$ almost surely
  - No assumption regarding lowest eigenvalues of H
  - Main result: $\boxed{\mathbb{E} f(\bar{\theta}_{n-1}) - f(\theta_*) \leqslant \dfrac{4\sigma^2 p}{n} + \dfrac{4R^2\|\theta_0 - \theta_*\|^2}{n}}$

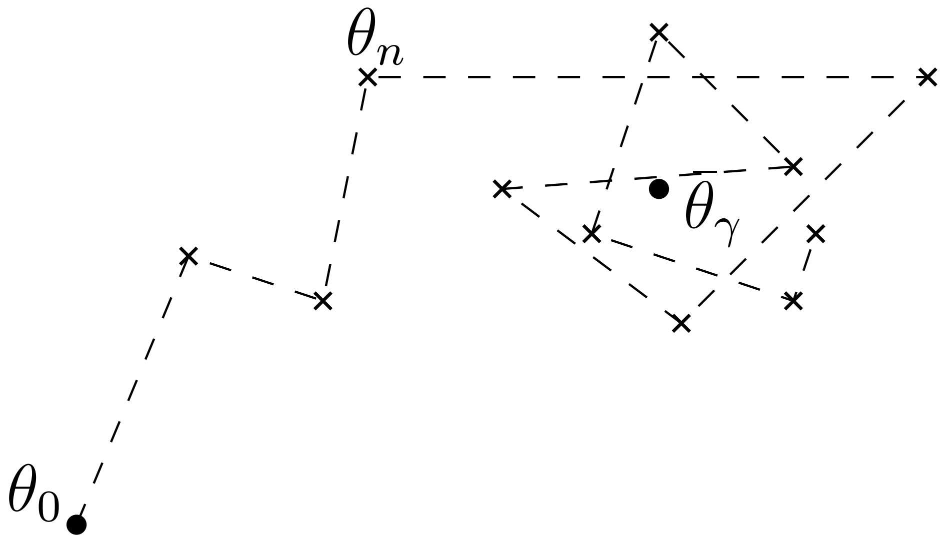
- **Matches statistical lower bound** (Tsybakov, 2003)
  - Non-asymptotic robust version of Györfi and Walk (1996)

Markov chain interpretation of constant step sizes

- LMS recursion for $f_n(\theta) = \frac{1}{2}\big(y_n - \langle \Phi(x_n), \theta\rangle\big)^2$

$$\theta_n = \theta_{n-1} - \gamma\big(\langle \Phi(x_n), \theta_{n-1}\rangle - y_n\big)\Phi(x_n)$$

- The sequence $(\theta_n)_n$ is a homogeneous Markov chain
  - convergence to a stationary distribution π_γ
  - with expectation $\bar{\theta}_\gamma \overset{\text{def}}{=} \int \theta \pi_\gamma(\mathrm{d}\theta)$



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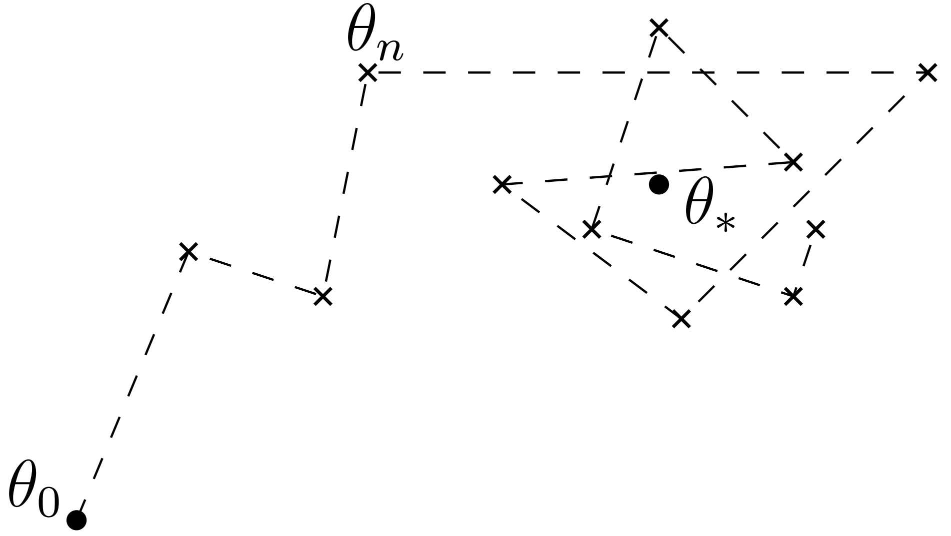
- **For least-squares, $\bar{\theta}_\gamma = \theta_*$**



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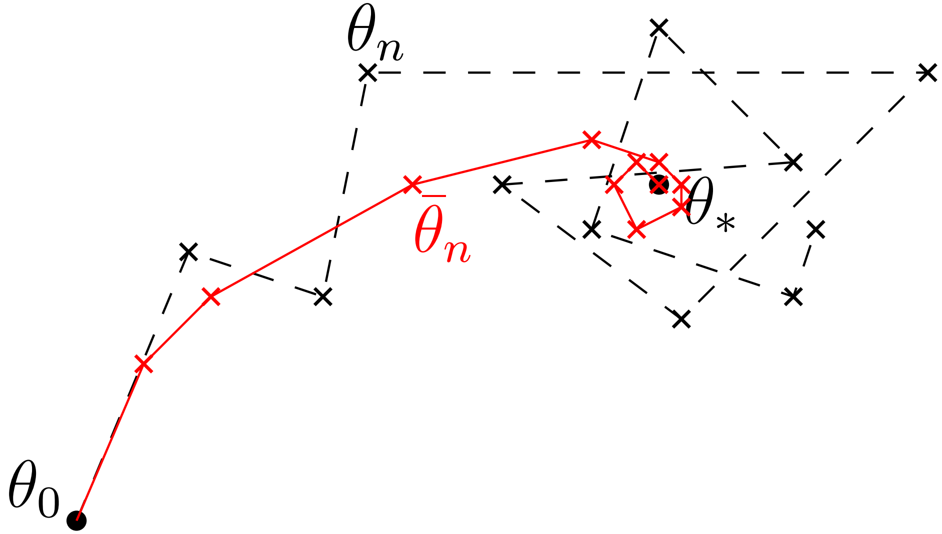

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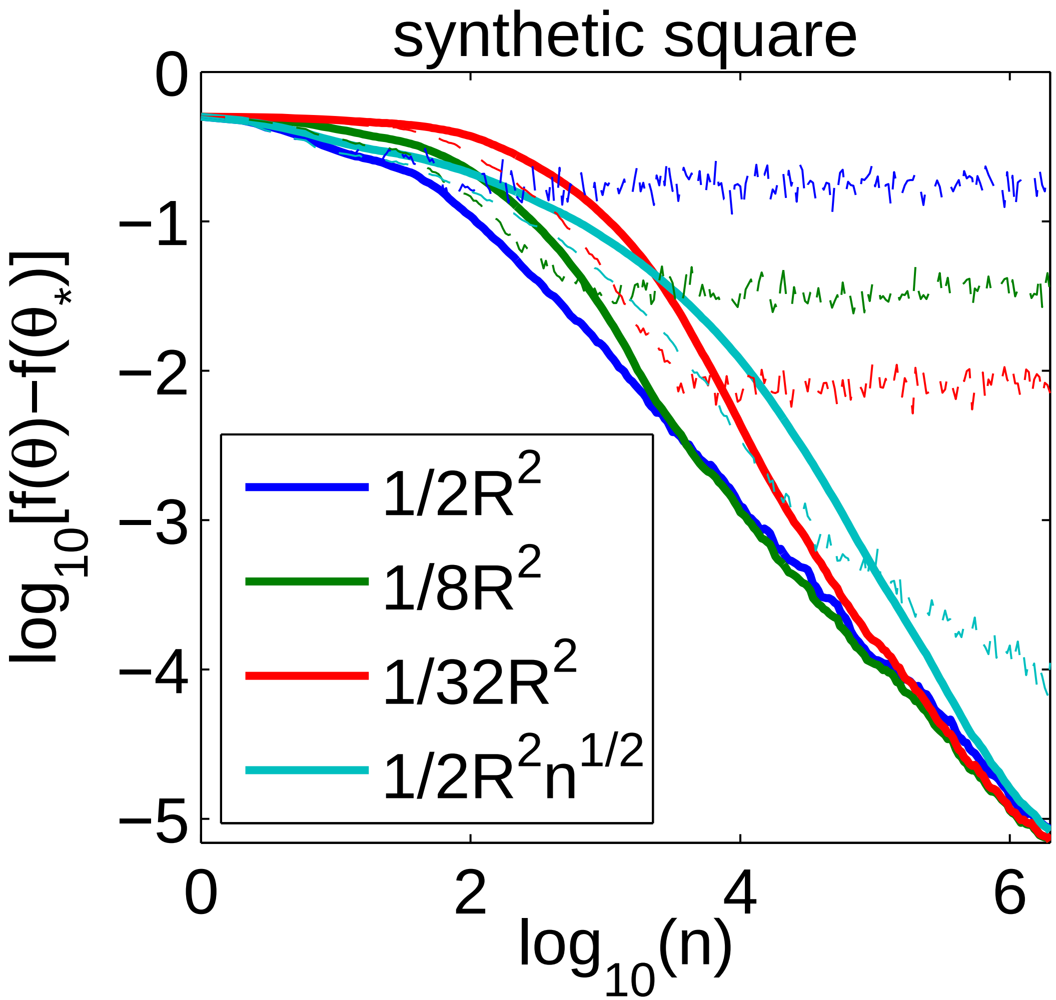
- **For least-squares, $\bar{\theta}_\gamma = \theta_*$**
  - θ_n does not converge to θ_* but oscillates around it
  - oscillations of order $\sqrt{\gamma}$

- **Ergodic theorem:**
  - Averaged iterates converge to $\bar{\theta}_\gamma = \theta_*$ at rate $O(1/n)$

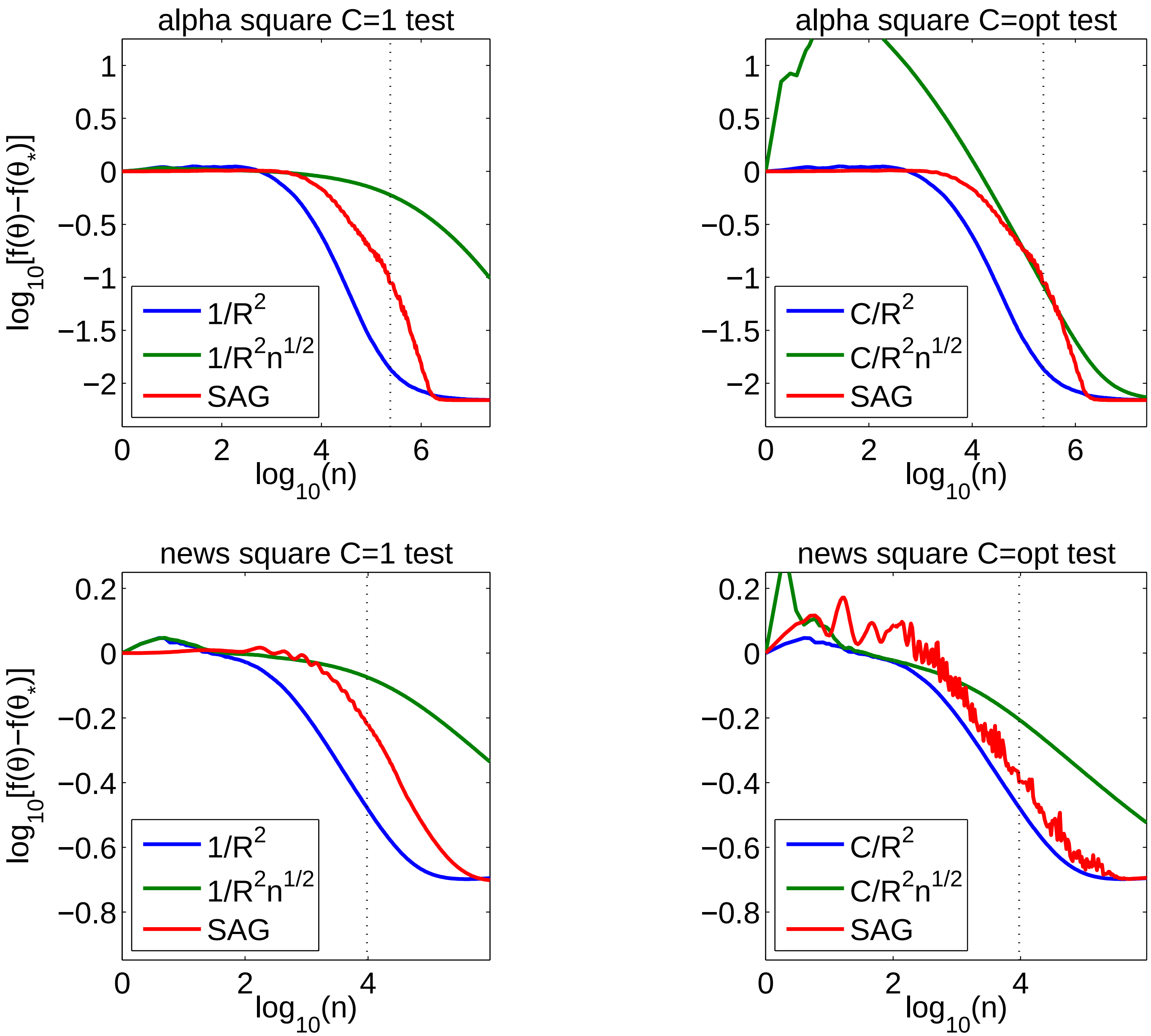
Simulations - synthetic examples

- Gaussian distributions - $p = 20$



Simulations - benchmarks

- *alpha* ($p = 500$, $n = 500\ 000$), *news* ($p = 1\ 300\ 000$, $n = 20\ 000$)



Beyond least-squares - Markov chain interpretation

- Recursion $\theta_n = \theta_{n-1} - \gamma f_n'(\theta_{n-1})$ also defines a Markov chain
  - Stationary distribution π_γ such that $\int f'(\theta)\pi_\gamma(\mathrm{d}\theta) = 0$
  - When f' is not linear, $f'(\int \theta\pi_\gamma(\mathrm{d}\theta)) \neq \int f'(\theta)\pi_\gamma(\mathrm{d}\theta) = 0$

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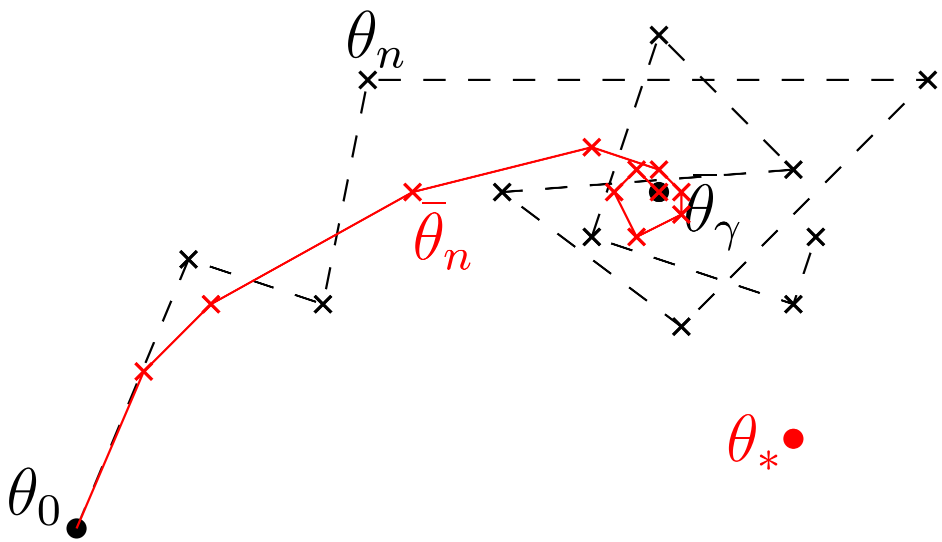
- **θ_n oscillates around the wrong value $\bar{\theta}_\gamma \neq \theta_*$**



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- θ_n **oscillates around the wrong value** $\bar{\theta}_\gamma \neq \theta_*$
  - moreover, $\|\theta_* - \theta_n\| = O_p(\sqrt{\gamma})$

- **Ergodic theorem**
  - averaged iterates converge to $\bar{\theta}_\gamma \neq \theta_*$ at rate $O(1/n)$
  - moreover, $\|\theta_* - \bar{\theta}_\gamma\| = O(\gamma)$ (Bach, 2013)

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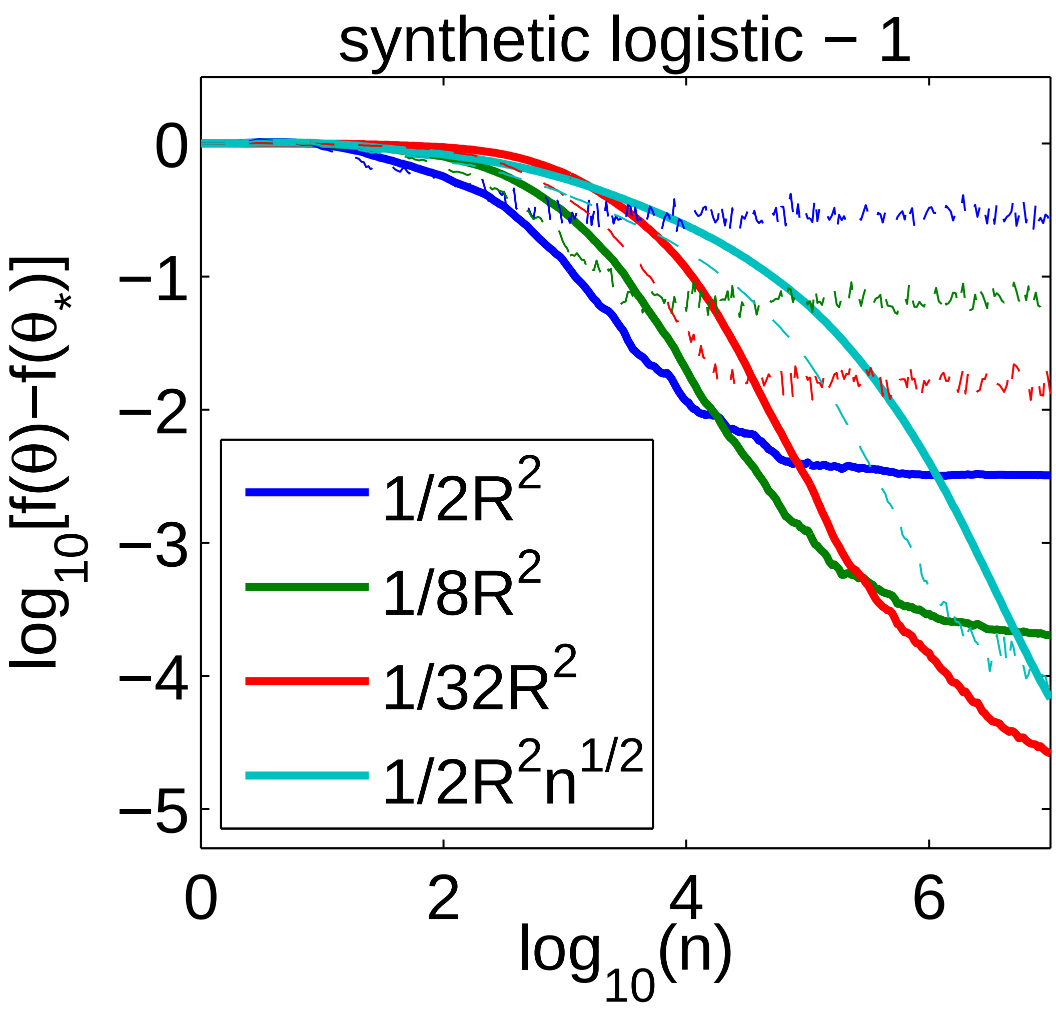

Restoring convergence through online Newton steps

- **Known facts**

  1. Averaged SGD with $\gamma_n \propto n^{-1/2}$ leads to *robust* rate $O(n^{-1/2})$ for all convex functions
  2. Averaged SGD with γ_n constant leads to *robust* rate $O(n^{-1})$ for all convex *quadratic* functions
  3. Newton's method squares the error at each iteration for smooth functions
  4. A single step of Newton's method is equivalent to minimizing the quadratic Taylor expansion

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- **Online Newton step**

  – Rate: $O((n^{-1/2})^2 + n^{-1}) = O(n^{-1})$
  – Complexity: $O(p)$ per iteration

Restoring convergence through online Newton steps

- The Newton step for $f = \mathbb{E} f_n(\theta) \stackrel{\text{def}}{=} \mathbb{E}\big[\ell(y_n, \langle\theta, \Phi(x_n)\rangle)\big]$ at $\tilde\theta$ is equivalent to minimizing the quadratic approximation

$$
\begin{aligned}
g(\theta) &= f(\tilde\theta) + \langle f'(\tilde\theta), \theta - \tilde\theta\rangle + \tfrac{1}{2}\langle \theta - \tilde\theta, f''(\tilde\theta)(\theta - \tilde\theta)\rangle \\
&= f(\tilde\theta) + \langle \mathbb{E} f_n'(\tilde\theta), \theta - \tilde\theta\rangle + \tfrac{1}{2}\langle \theta - \tilde\theta, \mathbb{E} f_n''(\tilde\theta)(\theta - \tilde\theta)\rangle \\
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- **Complexity of least-mean-square recursion for g is $O(p)$**

$$\theta_n = \theta_{n-1} - \gamma\big[f_n'(\tilde{\theta}) + f_n''(\tilde{\theta})(\theta_{n-1} - \tilde{\theta})\big]$$

  - $f_n''(\tilde{\theta}) = \ell''(y_n, \langle \tilde{\theta}, \Phi(x_n)\rangle)\Phi(x_n) \otimes \Phi(x_n)$ has rank one
  - New online Newton step without computing/inverting Hessians

Choice of support point for online Newton step

- **Two-stage procedure**

(1) Run $n/2$ iterations of averaged SGD to obtain $\tilde{\theta}$
(2) Run $n/2$ iterations of averaged constant step-size LMS

  - Reminiscent of one-step estimators (see, e.g., Van der Vaart, 2000)
  - Provable convergence rate of $O(p/n)$ for logistic regression
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- **Update at each iteration using the current averaged iterate**

  - Recursion: $\boxed{\theta_n = \theta_{n-1} - \gamma\big[f_n'(\bar{\theta}_{n-1}) + f_n''(\bar{\theta}_{n-1})(\theta_{n-1} - \bar{\theta}_{n-1})\big]}$
  - No provable convergence rate (yet) but best practical behavior
  - Note (dis)similarity with regular SGD: $\theta_n = \theta_{n-1} - \gamma f_n'(\theta_{n-1})$

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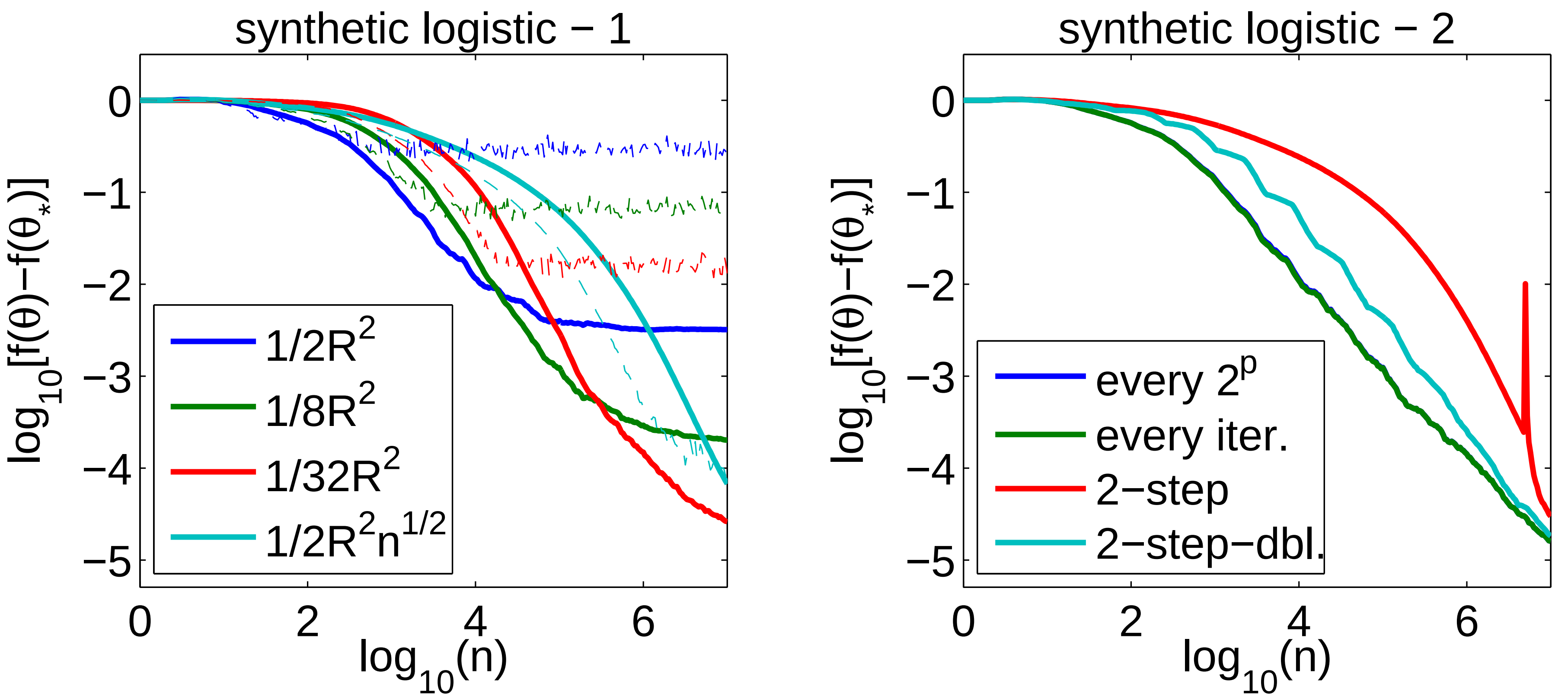

Simulations - benchmarks

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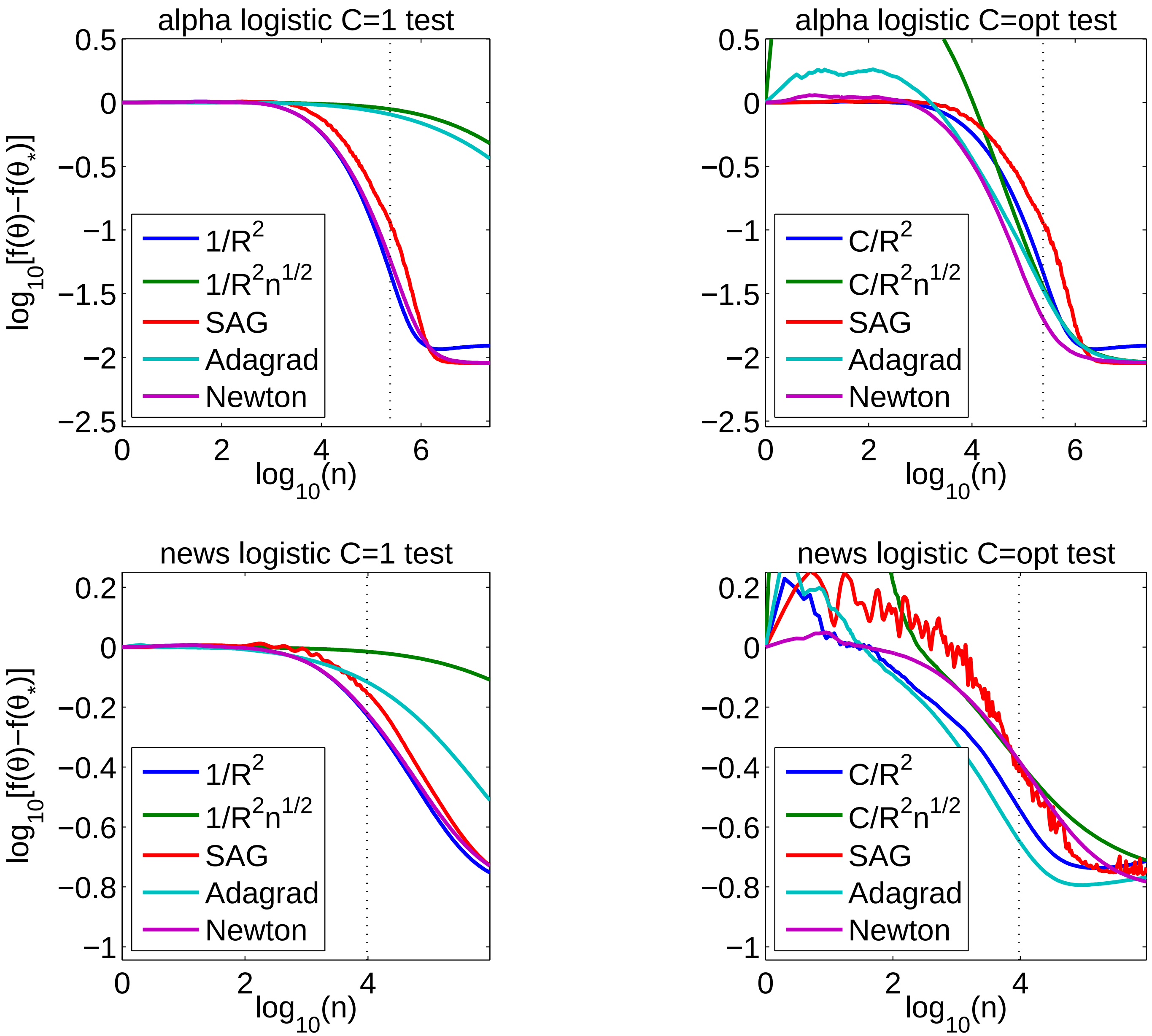

Conclusions

- **Constant-step-size averaged stochastic gradient descent**
  - Reaches convergence rate $O(1/n)$ in all regimes
  - Improves on the $O(1/\sqrt{n})$ lower-bound of non-smooth problems
  - Efficient online Newton step for non-quadratic problems
  - Robustness to step-size selection

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- **Extensions and future work**
  - Going beyond a single pass
  - Pre-conditioning
  - Proximal extensions fo non-differentiable terms
  - kernels and non-parametric estimation
  - line-search
  - parallelization
  - Non-convex problems

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