# Stochastic gradient descent and robustness to ill-conditioning

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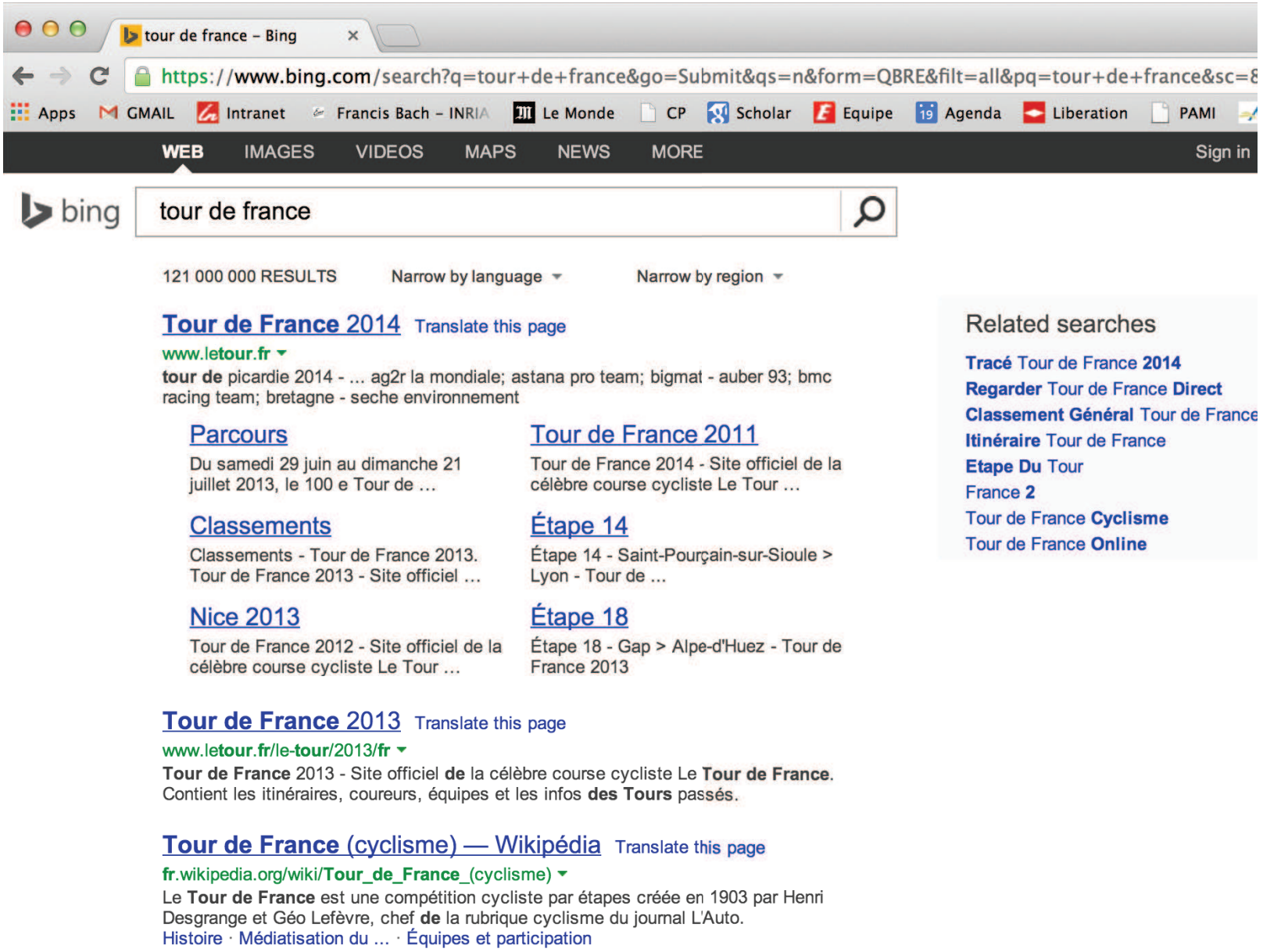
Joint work with Aymeric Dieuleveut, Nicolas Flammarion, Eric Moulines - Ecole des Ponts, June 2016

# "Big data" revolution?
# A new scientific context

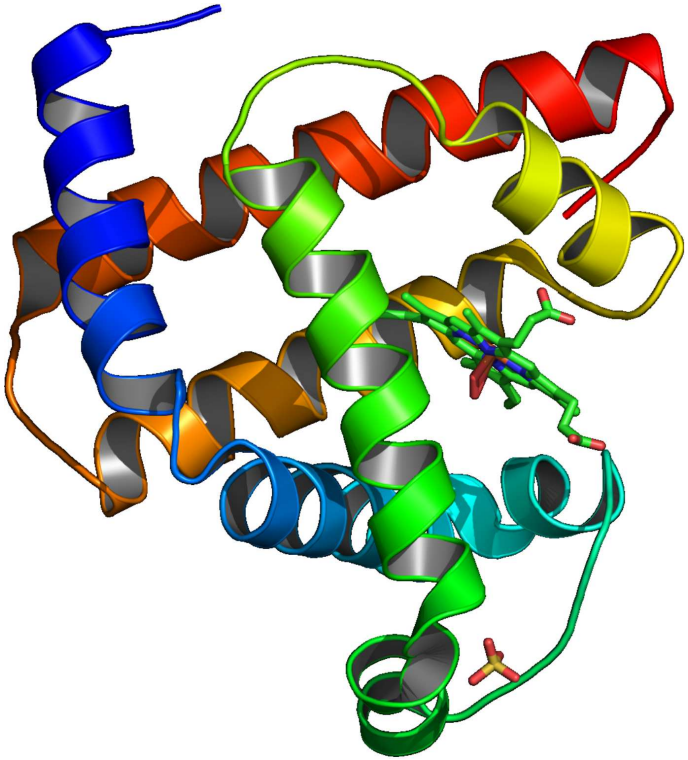
- **Data everywhere**: size does not (always) matter
- **Science and industry**
- **Size and variety**
- **Learning from examples**
  - $n$ observations in dimension $p$

# Search engines - Advertising



# Visual object recognition

# Bioinformatics



- **Protein**: Crucial elements of cell life
- **Massive data**: 2 millions for humans
- **Complex data**

# 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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- **Ideal running-time complexity**: $O(pn)$

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- **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 $\Phi(x) \in \mathbb{R}^p$
  - Explicit features adapted to inputs (can be learned as well)
  - Using Hilbert spaces for non-linear / non-parametric estimation

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- **(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

# Usual losses

- **Regression**: $y \in \mathbb{R}$, prediction $\hat{y} = \langle \theta, \Phi(x) \rangle$
  - quadratic loss $\frac{1}{2}(y - \hat{y})^2 = \frac{1}{2}(y - \langle \theta, \Phi(x) \rangle)^2$

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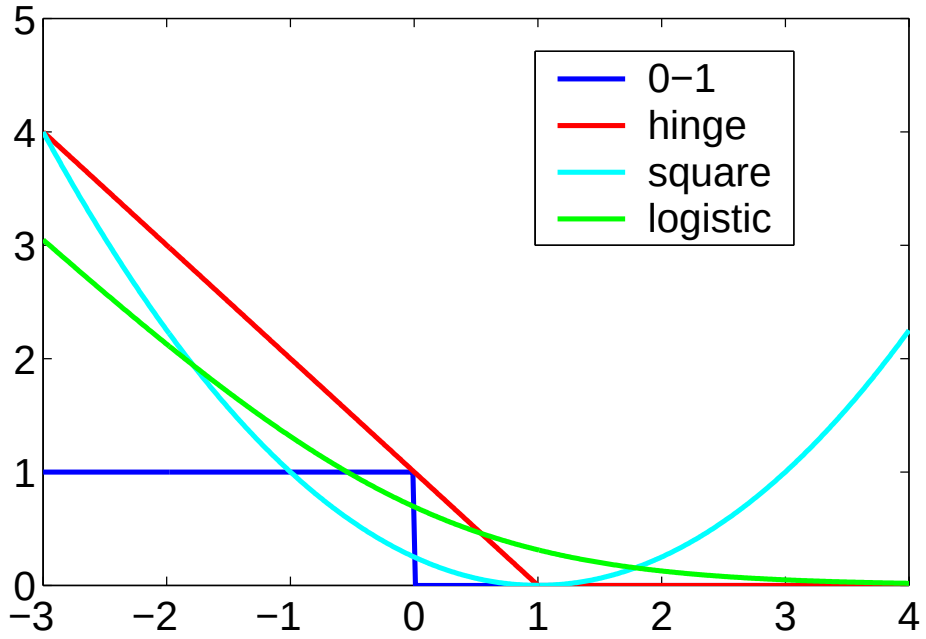
- **Classification** : $y \in \{-1, 1\}$, prediction $\hat{y} = \text{sign}(\langle \theta, \Phi(x) \rangle)$
  - loss of the form $\ell(y \langle \theta, \Phi(x) \rangle)$
  - "True" 0-1 loss: $\ell(y \langle \theta, \Phi(x) \rangle) = 1_{y \langle \theta, \Phi(x) \rangle < 0}$
  - Usual convex losses:



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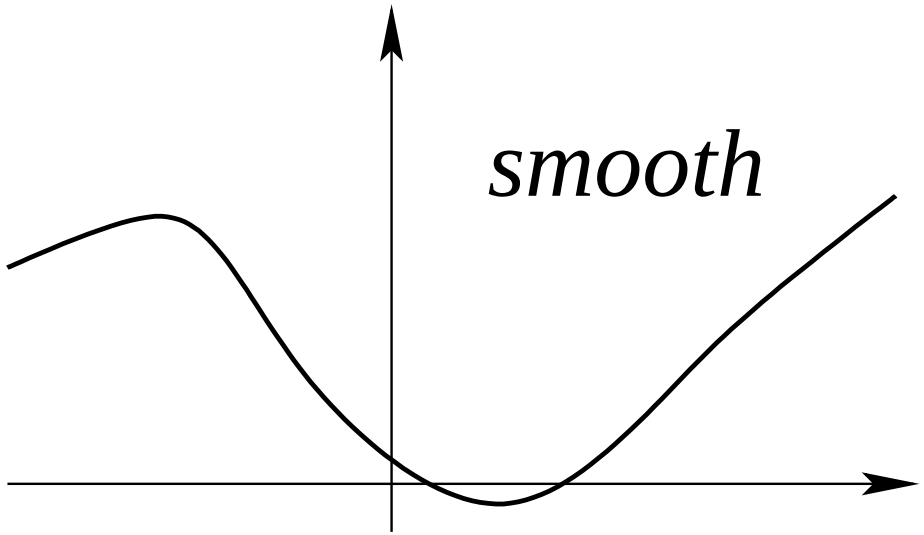
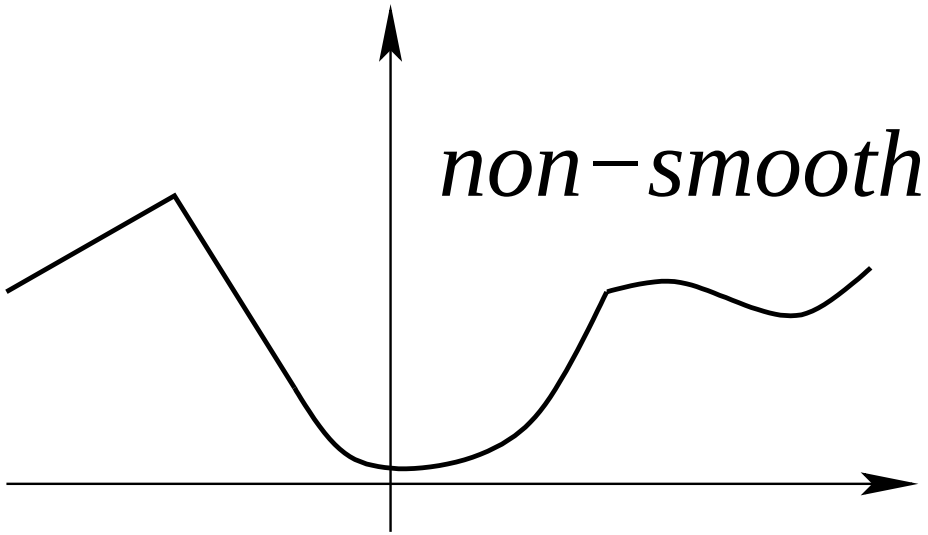
- Empirical risk: $\hat{f}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, \langle \theta, \Phi(x_i) \rangle)$ training cost
- Expected risk: $f(\theta) = \mathbb{E}_{(x,y)} \ell(y, \langle \theta, \Phi(x) \rangle)$ testing cost
- **Two fundamental questions**: (1) computing $\hat{\theta}$ and (2) analyzing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

# 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

$$\forall \theta \in \mathbb{R}^p, \text{ eigenvalues}\big[g''(\theta)\big] \leqslant L$$



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  - Hessian $\approx$ covariance matrix $\frac{1}{n} \sum_{i=1}^n \Phi(x_i) \otimes \Phi(x_i)$
  - Bounded data: $\|\Phi(x)\| \leqslant R \Rightarrow L = O(R^2)$

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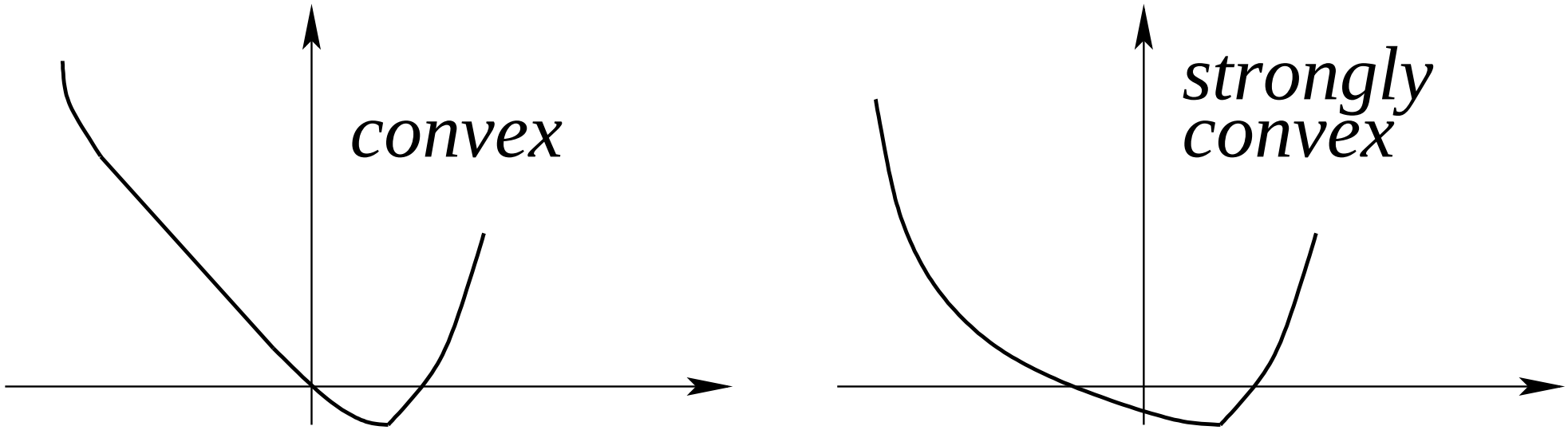

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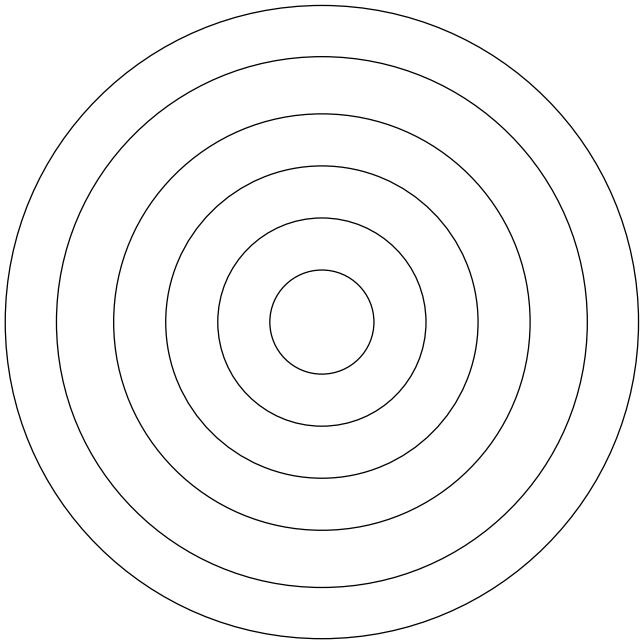
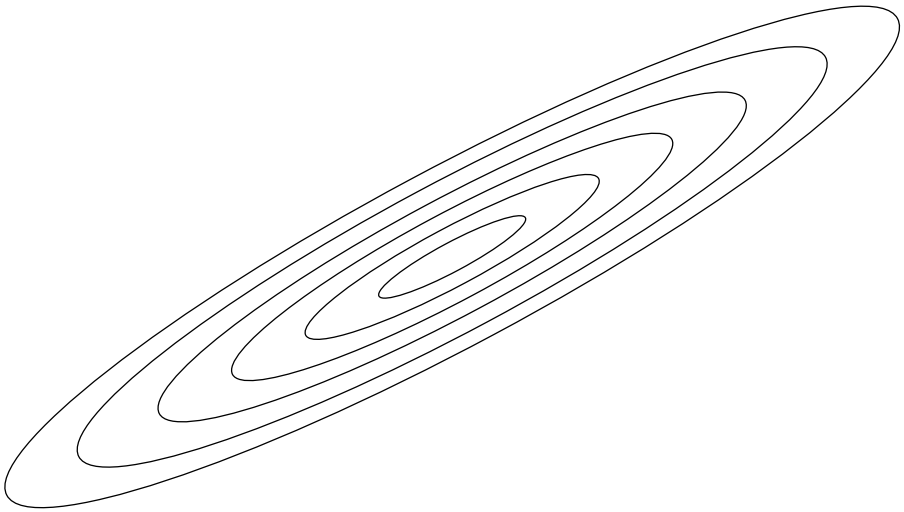


(large $\mu/L$)



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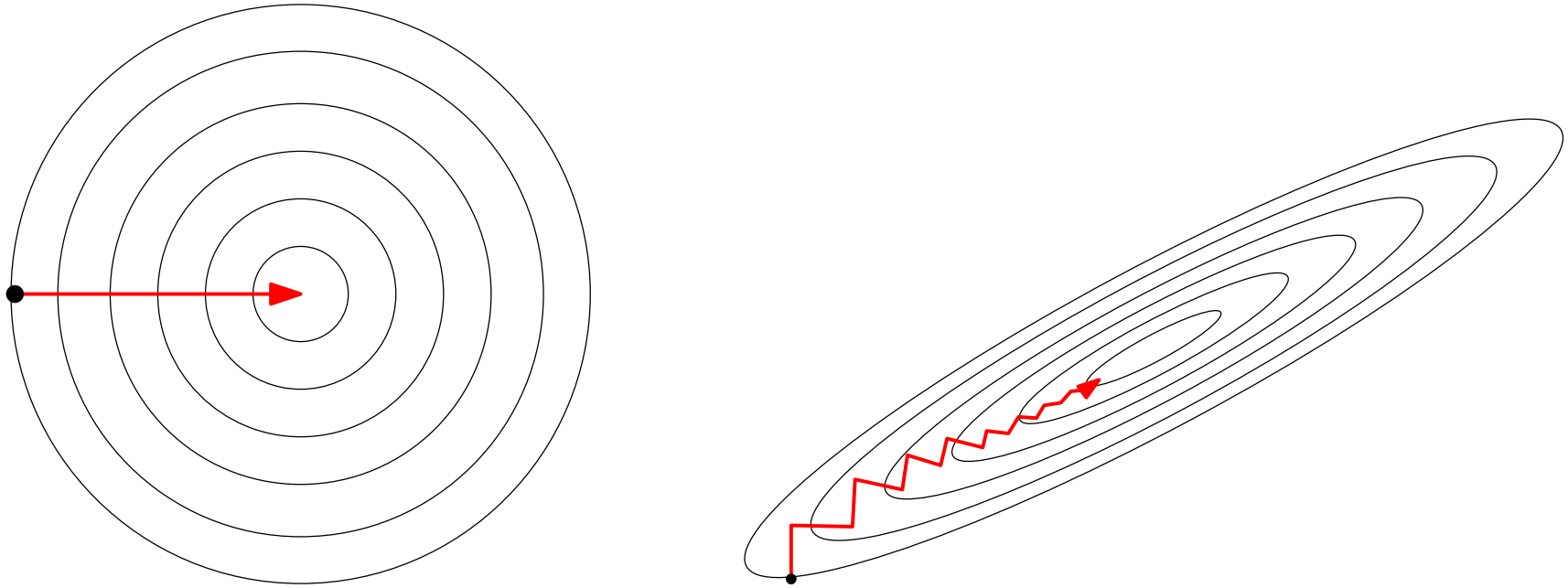
- **Adding regularization by $\frac{\mu}{2}\|\theta\|^2$**
  - creates additional bias unless $\mu$ is small

# 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
  - $O(e^{-(\mu/L)t})$ 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 $\theta_n \in \mathbb{R}^p$

# 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 $\theta_n \in \mathbb{R}^p$

- **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 $\gamma_n$? 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 analysis

- **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)
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- **A single algorithm for smooth problems with global 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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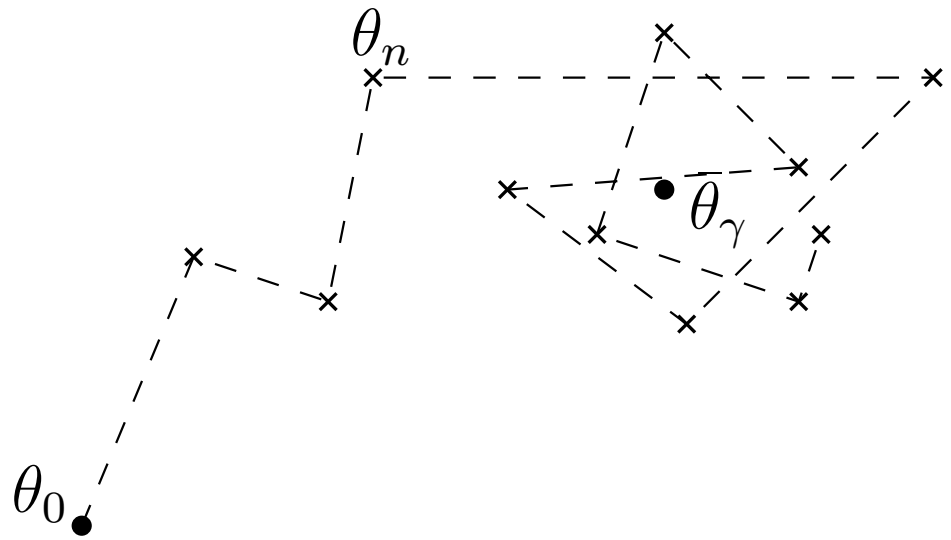
- **New analysis for averaging and constant step-size** $\gamma = 1/(4R^2)$
  - Assume $\|\Phi(x_n)\| \leqslant R$ and $|y_n - \langle \Phi(x_n), \theta_* \rangle| \leqslant \sigma$ almost surely
  - No assumption regarding lowest eigenvalues of $H$
  - Main result: $\boxed{\mathbb{E} f(\bar{\theta}_n) - f(\theta_*) \leqslant \dfrac{4\sigma^2 p}{n} + \dfrac{4R^2 \|\theta_0 - \theta_*\|^2}{n}}$
- **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 $\pi_\gamma$
  - with expectation $\bar{\theta}_\gamma \stackrel{\text{def}}{=} \int \theta \pi_\gamma(\mathrm{d}\theta)$



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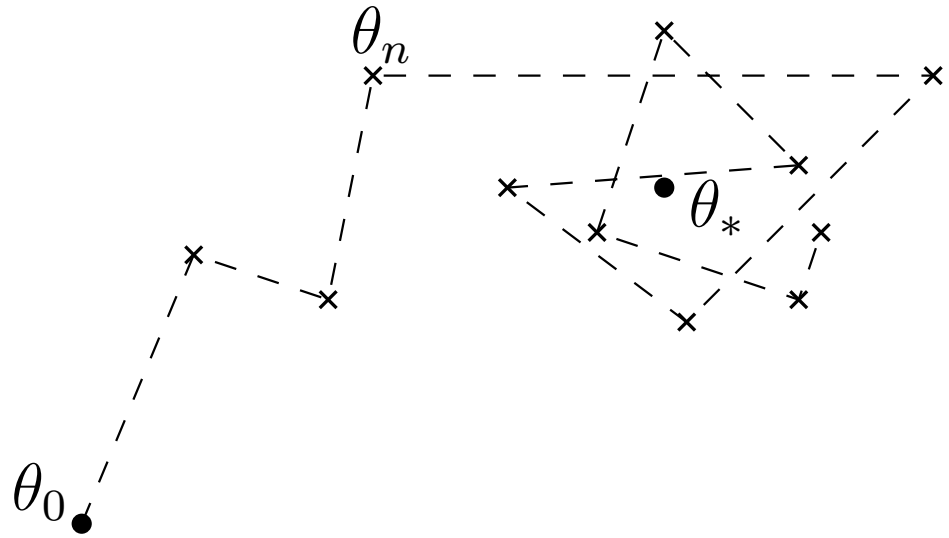

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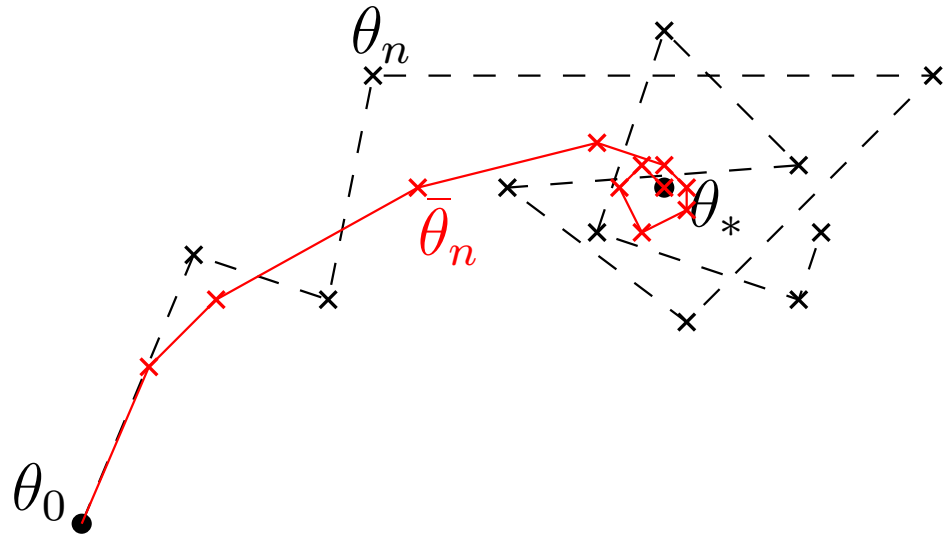

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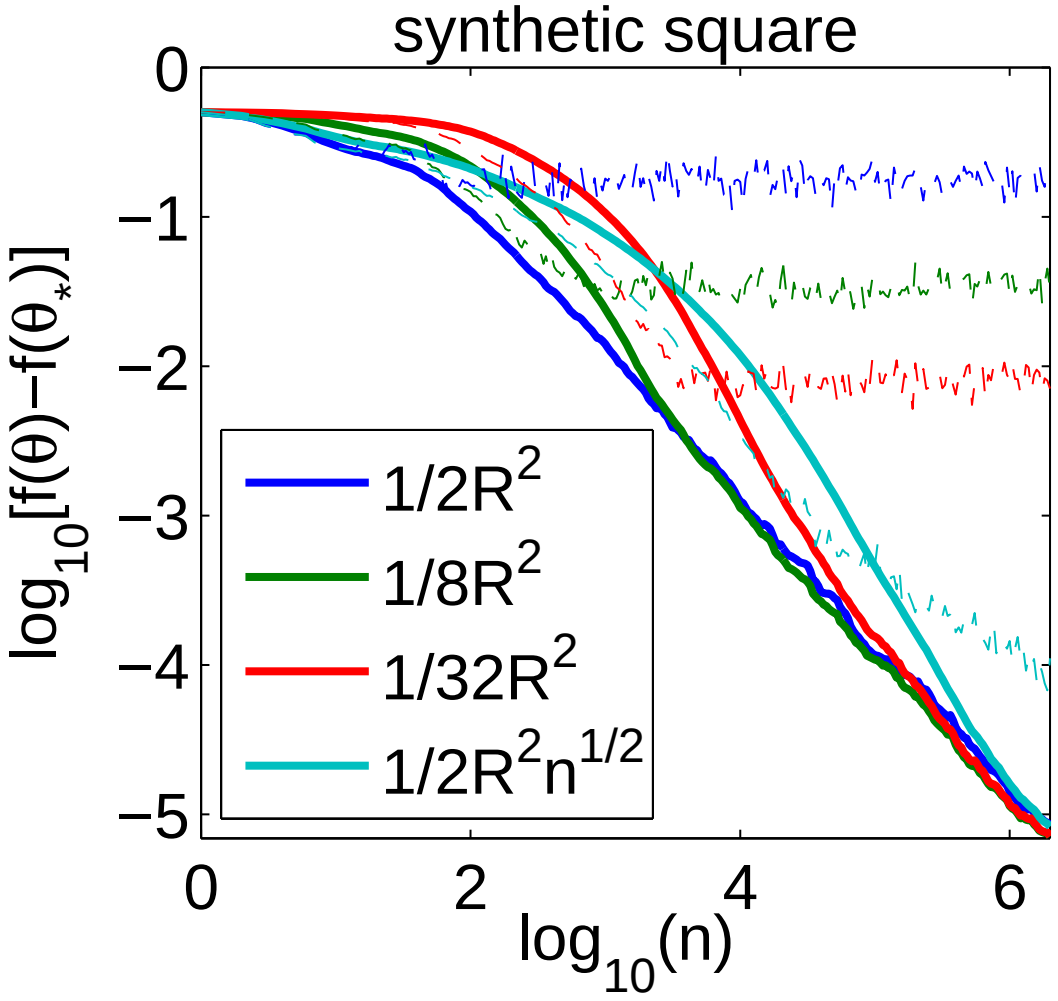
- **For least-squares, $\bar{\theta}_\gamma = \theta_*$**
  - $\theta_n$ does not converge to $\theta_*$ but oscillates around it
  - oscillations of order $\sqrt{\gamma}$
- **Ergodic theorem:**
  - Averaged iterates converge to $\bar{\theta}_\gamma = \theta_*$ at rate $O(1/n)$

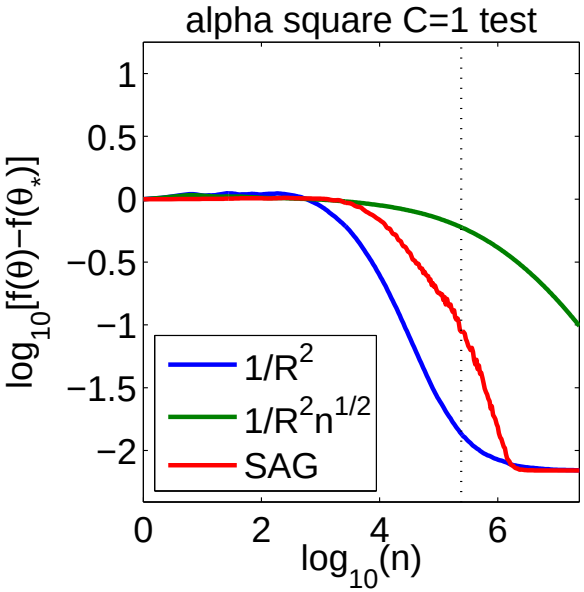
# Simulations - synthetic examples

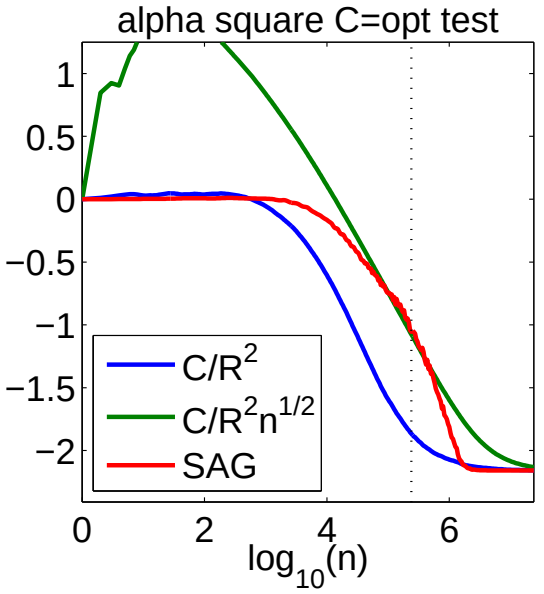
- Gaussian distributions - $p = 20$

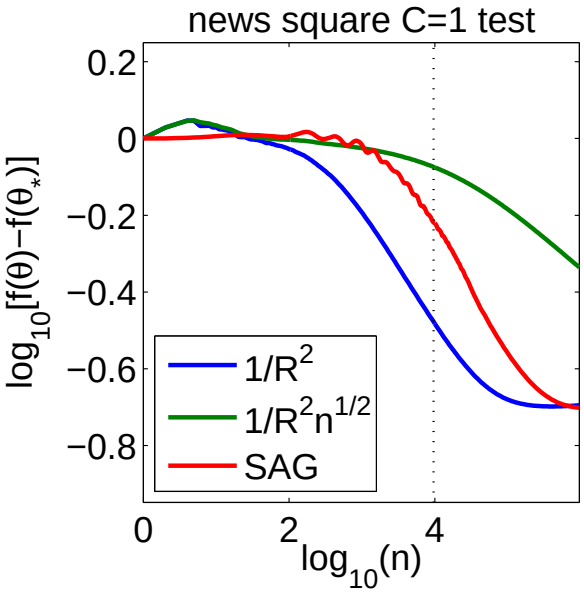


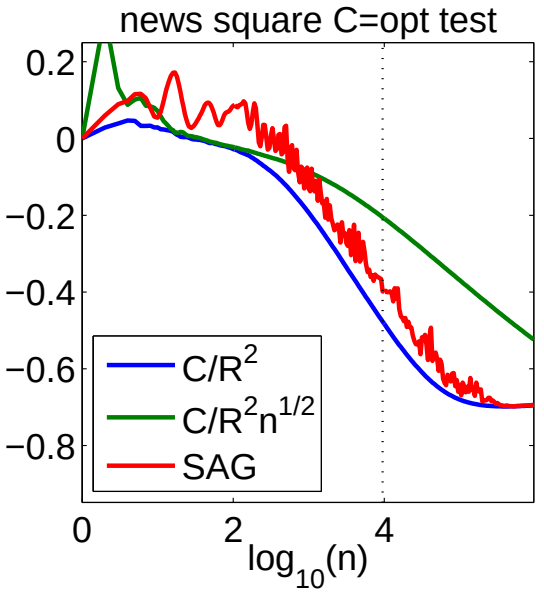
# Simulations - benchmarks

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



# Isn't least-squares regression a "regression"?

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- **Least-squares regression**
  - Simpler to analyze and understand
  - Explicit relationship to bias/variance trade-offs (next slides)
- **Many important loss functions are not quadratic**
  - Beyond least-squares with online Newton steps
  - Complexity of $O(p)$ per iteration with rate $O(p/n)$
  - See Bach and Moulines (2013) for details

# Optimal bounds for least-squares?

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- **Refined analysis** (Défossez and Bach, 2015)

$$\mathbb{E} f(\bar{\theta}_n) - f(\theta_*) \leqslant \frac{\sigma^2 p}{n} + \frac{\|H^{-1/2}(\theta_0 - \theta_*)\|_2^2}{\gamma^2 n^2}$$

  - In practice: bias may be larger than variance, $\sigma^2 p/n$ pessimistic

# Optimal bounds for least-squares?

- **Least-squares**: cannot beat $\sigma^2 p/n$ (Tsybakov, 2003). Really?

- **Refined analysis** (Défossez and Bach, 2015)

$$\mathbb{E} f(\bar{\theta}_n) - f(\theta_*) \leqslant \frac{\sigma^2 p}{n} + \frac{\|H^{-1/2}(\theta_0 - \theta_*)\|_2^2}{\gamma^2 n^2}$$

  - In practice: bias may be larger than variance, $\sigma^2 p/n$ pessimistic

- **Refined assumptions with adaptivity** (Dieuleveut and Bach, 2014)

$$\mathbb{E} f(\bar{\theta}_n) - f(\theta_*) \leqslant \frac{\sigma^2 \gamma^{1/\alpha} \operatorname{tr} H^{1/\alpha}}{n^{1-1/\alpha}} + \frac{\|H^{1/2-r}(\theta_0 - \theta_*)\|_2^2}{\gamma^{2r} n^{2\min\{r,1\}}}$$

  - SGD is adaptive to the covariance matrix eigenvalue decay
  - Leads to optimal rates for non-parametric regression

# Achieving optimal bias and variance terms

- **Current results with averaged SGD**
  - **Variance** (starting from optimal $\theta_*$) $= \dfrac{\sigma^2 p}{n}$
  - **Bias** (no noise) $= \min\left\{\dfrac{R^2\|\theta_0 - \theta_*\|^2}{n}, \dfrac{R^4\langle\theta_0 - \theta_*, H^{-1}(\theta_0 - \theta_*)\rangle}{n^2}\right\}$

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- **Acceleration is notoriously non-robust to noise** (d'Aspremont, 2008; Schmidt et al., 2011)
  - For non-structured noise, see Lan (2012)

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# 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 $\pi_\gamma$ 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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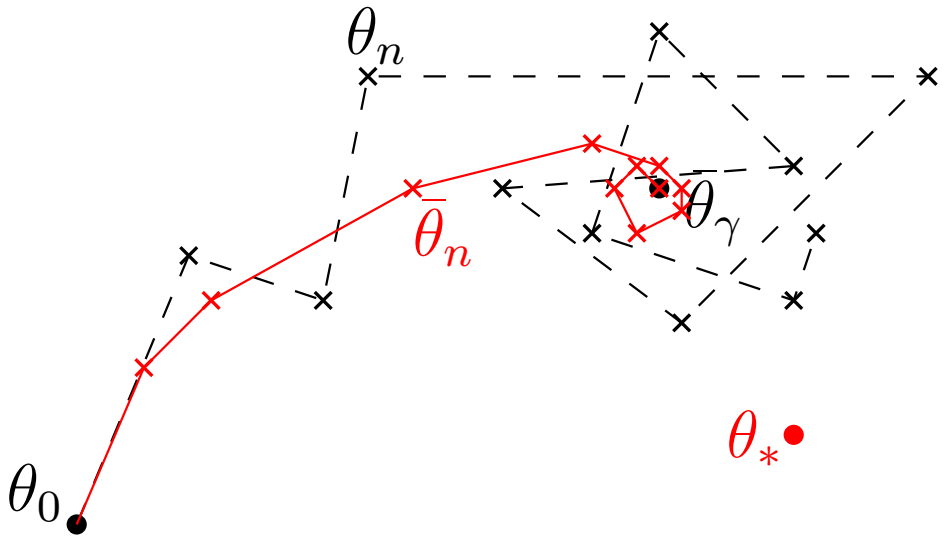

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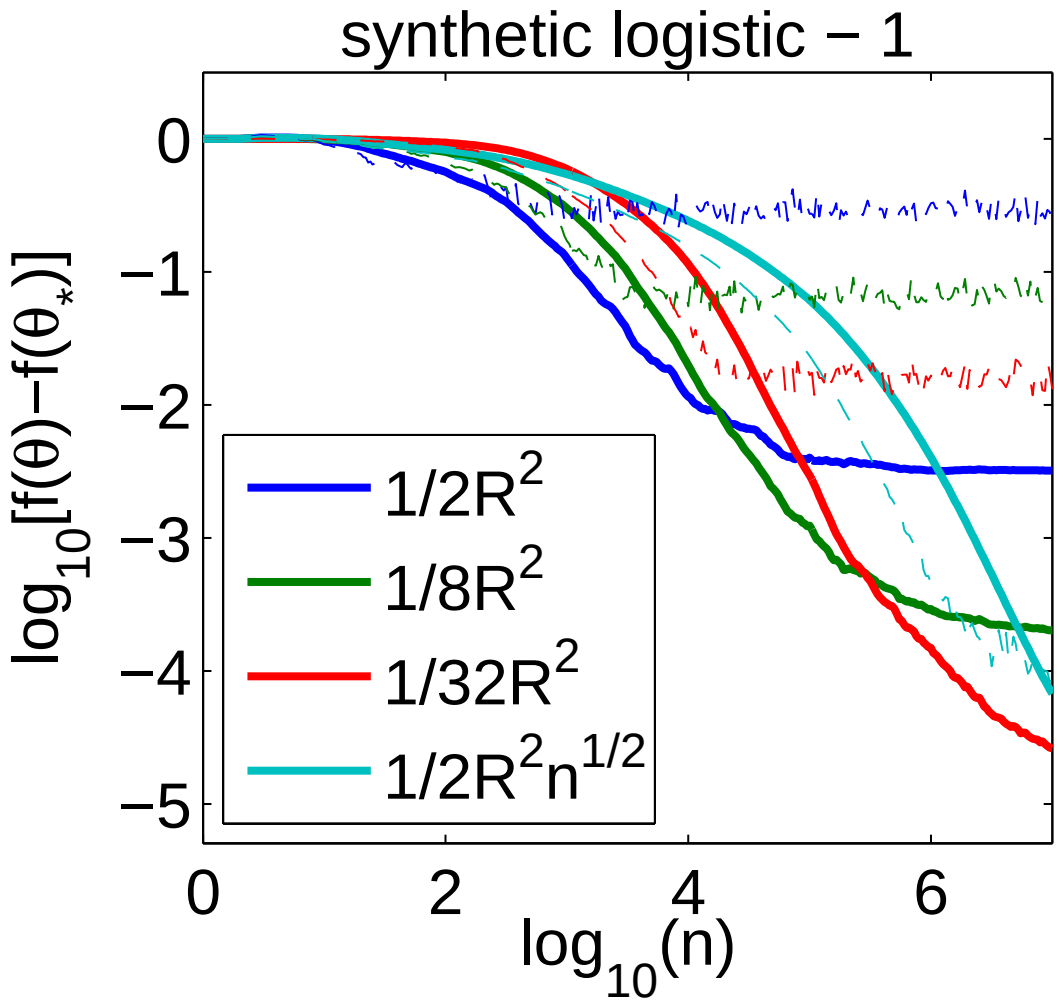
- **Ergodic theorem**
  - averaged iterates converge to $\bar{\theta}_\gamma \neq \theta_*$ at rate $O(1/n)$
  - moreover, $\|\theta_* - \bar{\theta}_\gamma\| = O(\gamma)$ (Bach, 2013)

# Simulations - synthetic examples

- Gaussian distributions - $p = 20$



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

- **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 \\
&= \mathbb{E}\Big[ f(\tilde{\theta}) + \langle f_n'(\tilde{\theta}), \theta - \tilde{\theta} \rangle + \tfrac{1}{2} \langle \theta - \tilde{\theta}, f_n''(\tilde{\theta})(\theta - \tilde{\theta}) \rangle \Big]
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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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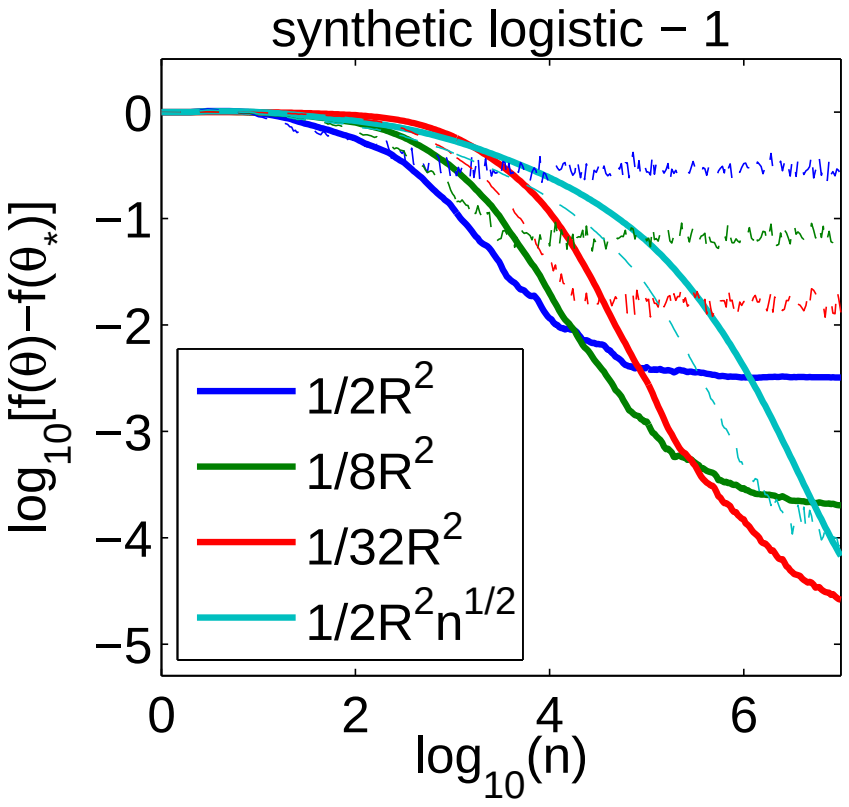
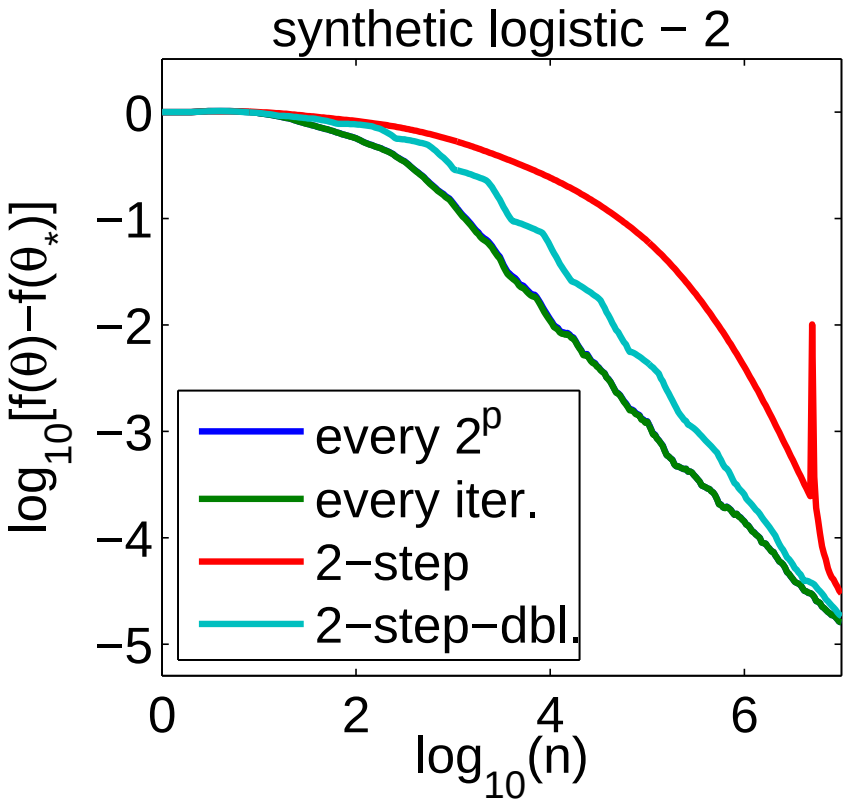
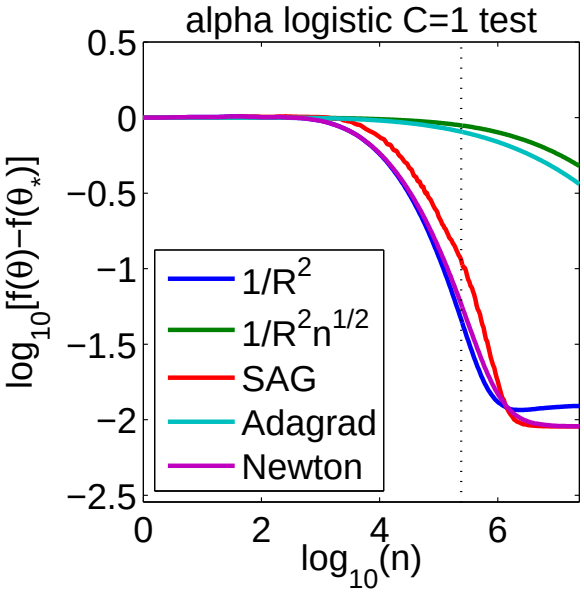
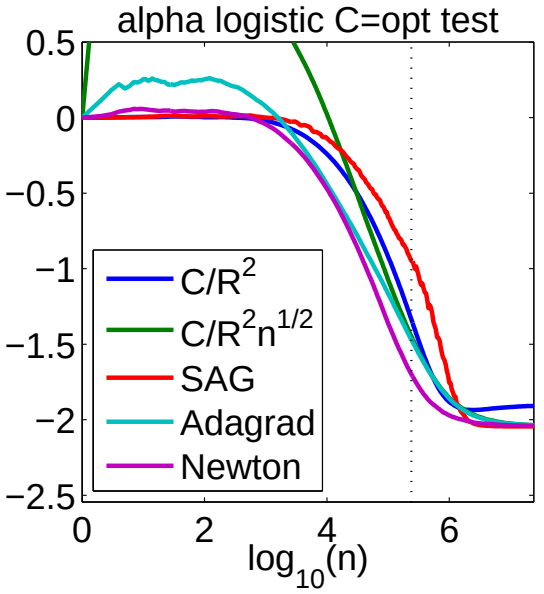


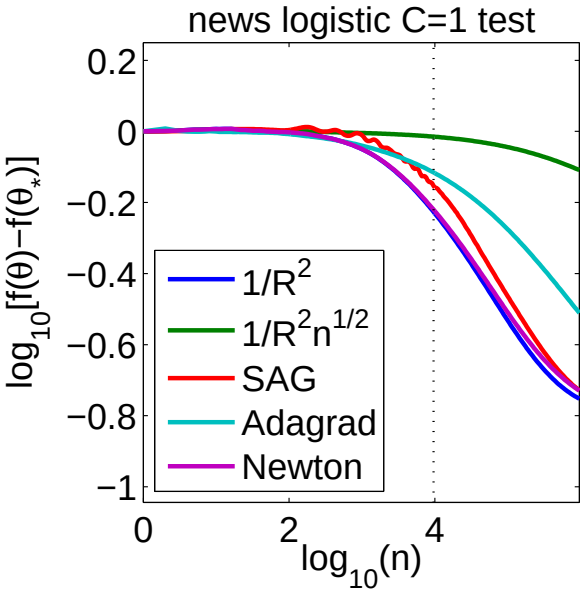



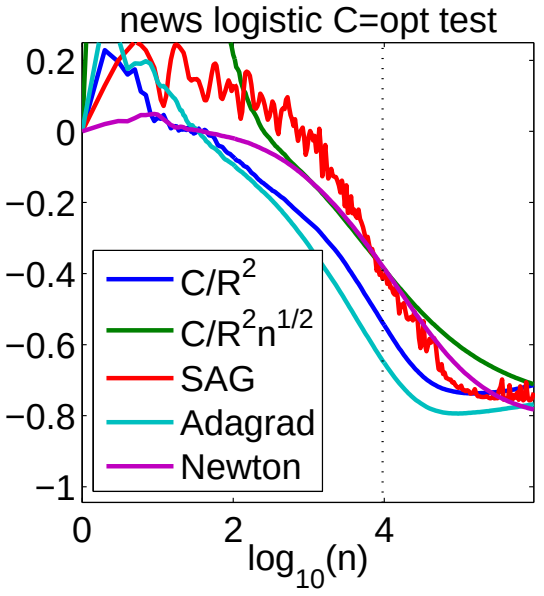
# Simulations - benchmarks

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



# 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 and adaptivity

# Conclusions

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- **Extensions and future work**
  - Going beyond a single pass (Le Roux, Schmidt, and Bach, 2012; Defazio, Bach, and Lacoste-Julien, 2014)
  - Proximal extensions fo non-differentiable terms
  - Kernels and nonparametric estimation (Dieuleveut and Bach, 2014)
  - Parallelization
  - Non-convex problems

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