Large Scale Machine Learning Over Networks

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Scientific context

- **Proliferation of digital data**
  - Personal data
  - Industry
  - Scientific: from bioinformatics to humanities

- **Need for automated processing of massive data**

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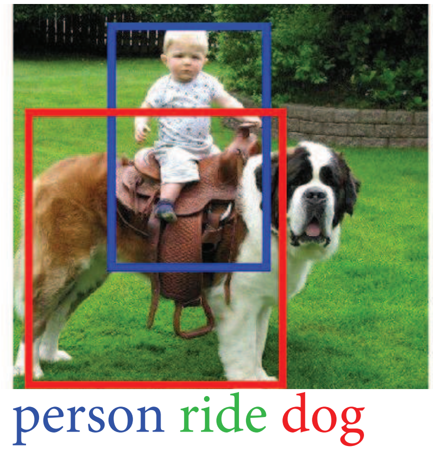
- **Series of "hypes"**

  Big data $\rightarrow$ Data science $\rightarrow$ Machine Learning
  $\rightarrow$ Deep Learning $\rightarrow$ Artificial Intelligence

Recent progress in perception (vision, audio, text)

From translate.google.fr



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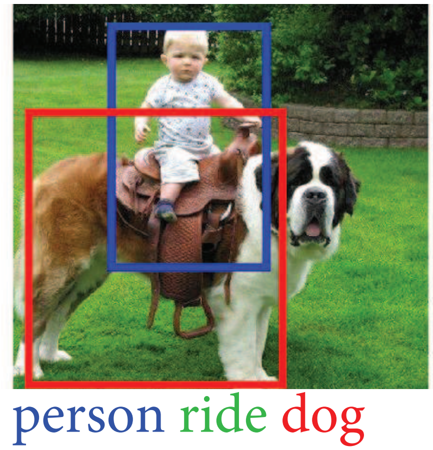

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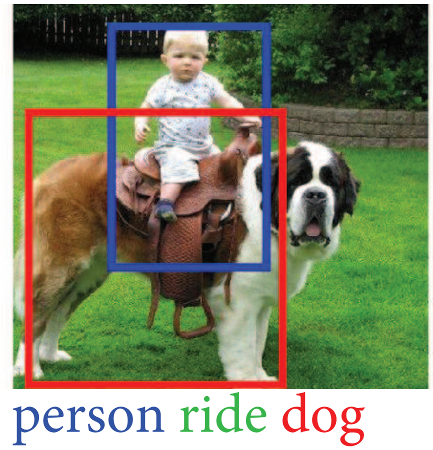

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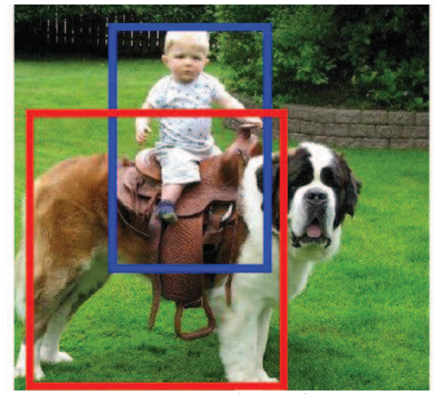

person ride dog

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Outline

1. **Parametric supervised learning on a single machine**
   - Machine learning $\approx$ optimization of finite sums
   - From batch to stochastic gradient methods
   - Linearly-convergent stochastic methods for convex problems

2. **Machine learning over networks**
   - Centralized and decentralized methods
   - From network averaging to optimization
   - Distributing the fastest single machine algorithms

Parametric supervised machine learning

- **Data**: n observations $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$, $i = 1, \dots, n$
- **Prediction function** $h(x, \theta) \in \mathbb{R}$ parameterized by $\theta \in \mathbb{R}^d$

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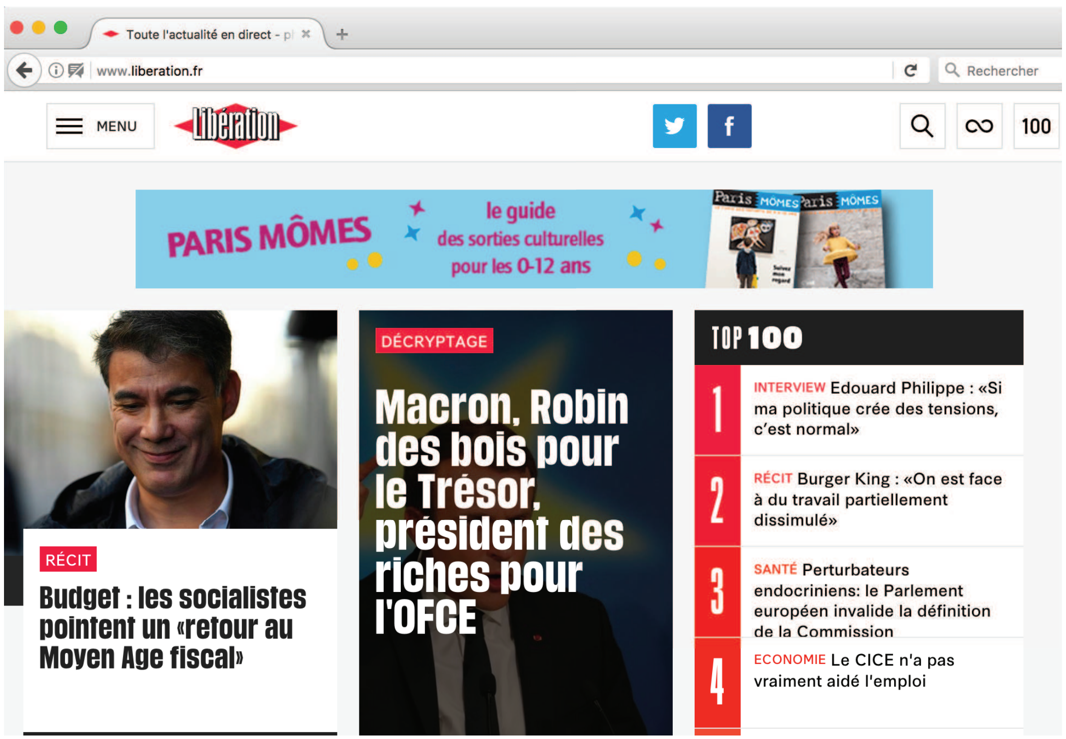

- **Advertising**: $n > 10^9$
  - $\Phi(x) \in \{0, 1\}^d$, $d > 10^9$
  - Navigation history + ad

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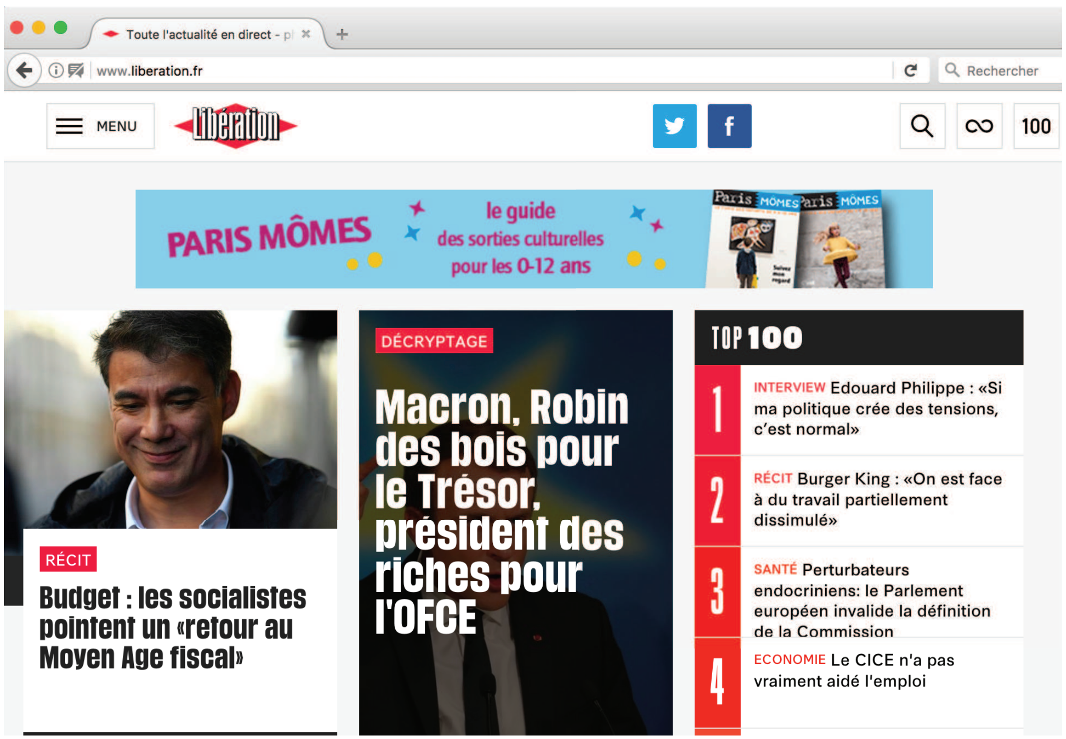

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- Linear predictions
  - $h(x, \theta) = \theta^\top \Phi(x)$

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x_1 x_2 x_3 x_4 x_5 x_6

$y_1 = 1$ $y_2 = 1$ $y_3 = 1$ $y_4 = -1$ $y_5 = -1$ $y_6 = -1$

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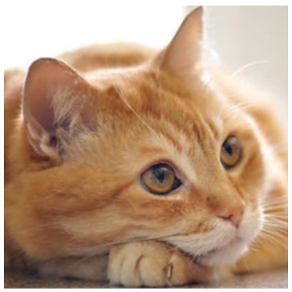		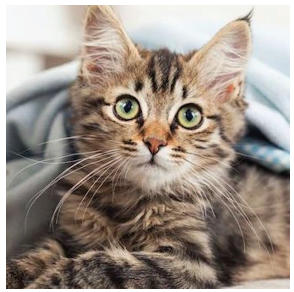			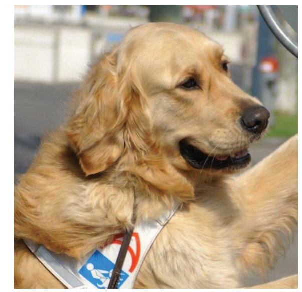
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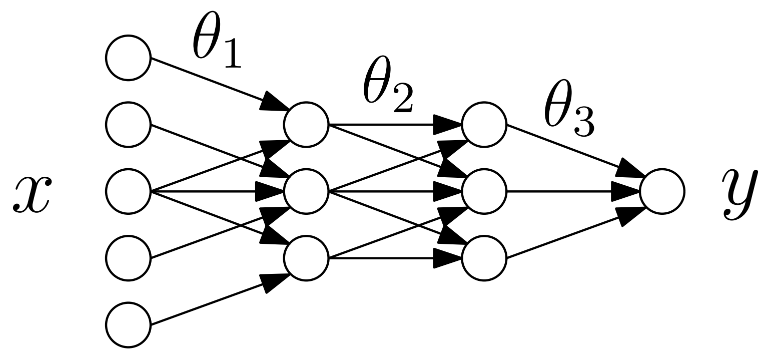
  - Neural networks ($n, d > 10^6$): $h(x, \theta) = \theta_m^\top \sigma(\theta_{m-1}^\top \sigma(\cdots \theta_2^\top \sigma(\theta_1^\top x))$



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- **Prediction function** $h(x, \theta) \in \mathbb{R}$ parameterized by $\theta \in \mathbb{R}^d$
- **(regularized) empirical risk minimization**:

$$\min_{\theta \in \mathbb{R}^d} \quad \frac{1}{n} \sum_{i=1}^{n} \ \ell\big(y_i, h(x_i, \theta)\big) \quad + \quad \lambda \Omega(\theta)$$

data fitting term + regularizer

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$$\min_{\theta \in \mathbb{R}^d} \quad \frac{1}{2n} \sum_{i=1}^{n} \big(y_i - h(x_i, \theta)\big)^2 \quad + \quad \lambda \Omega(\theta)$$

(least-squares regression)

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$$\min_{\theta \in \mathbb{R}^d} \quad \frac{1}{n} \sum_{i=1}^{n} \log\big(1 + \exp(-y_i h(x_i, \theta))\big) \quad + \quad \lambda \Omega(\theta)$$

(logistic regression)

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data fitting term $+$ regularizer

- Optimization: optimization of regularized risk training cost

Parametric supervised machine learning

- **Data**: n observations $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$, $i = 1, \dots, n$, **i.i.d.**

- **Prediction function** $h(x, \theta) \in \mathbb{R}$ parameterized by $\theta \in \mathbb{R}^d$

- **(regularized) empirical risk minimization**:

$$\min_{\theta \in \mathbb{R}^d} \quad \frac{1}{n} \sum_{i=1}^{n} \Big\{ \ell\big(y_i, h(x_i, \theta)\big) \quad + \quad \lambda \Omega(\theta) \Big\} \qquad = \frac{1}{n} \sum_{i=1}^{n} f_i(\theta)$$

data fitting term $+$ regularizer

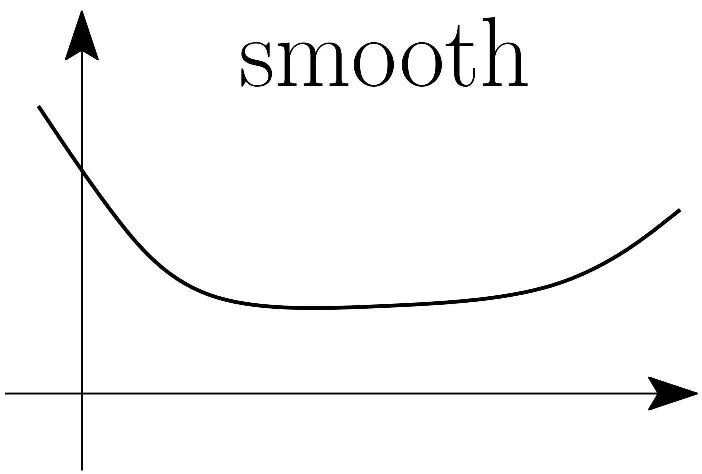
- Optimization: optimization of regularized risk — training cost

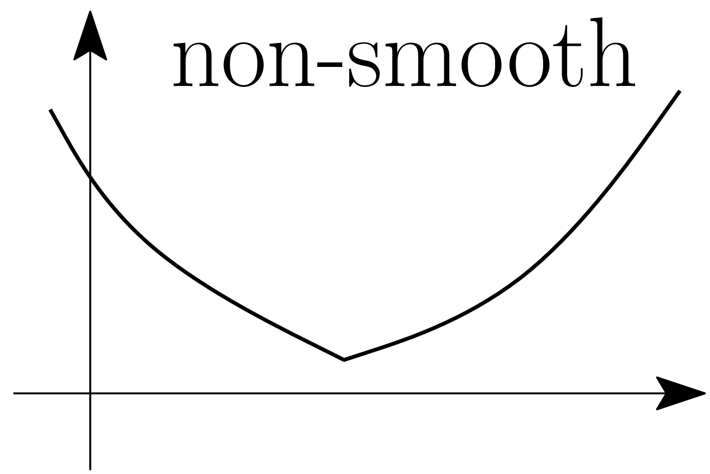
- Statistics: guarantees on $\mathbb{E}_{p(x,y)} \ell(y, h(x, \theta))$ — testing cost

Smoothness and (strong) convexity

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

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





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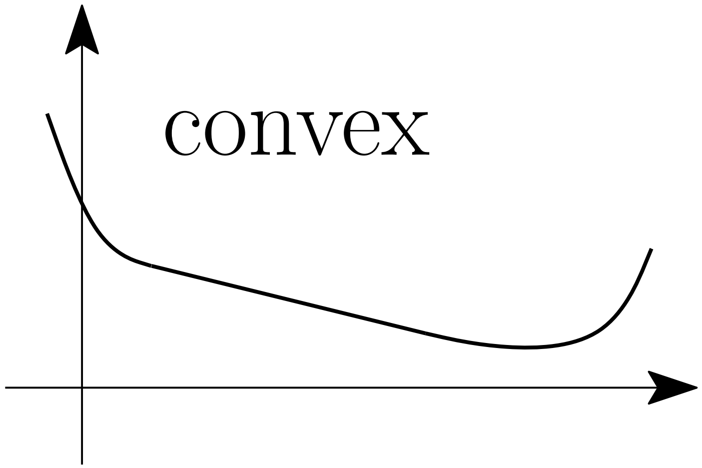
- **Machine learning**
  - with $g(\theta) = \frac{1}{n}\sum_{i=1}^n \ell(y_i, h(x_i, \theta))$
  - Smooth prediction function $\theta \mapsto h(x_i, \theta)$ + smooth loss

Smoothness and (strong) convexity

- A twice differentiable function $g : \mathbb{R}^d \to \mathbb{R}$ is convex if and only if
$$\forall \theta \in \mathbb{R}^d,\ \text{eigenvalues}\big[g''(\theta)\big] \geqslant 0$$



Smoothness and (strong) convexity

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

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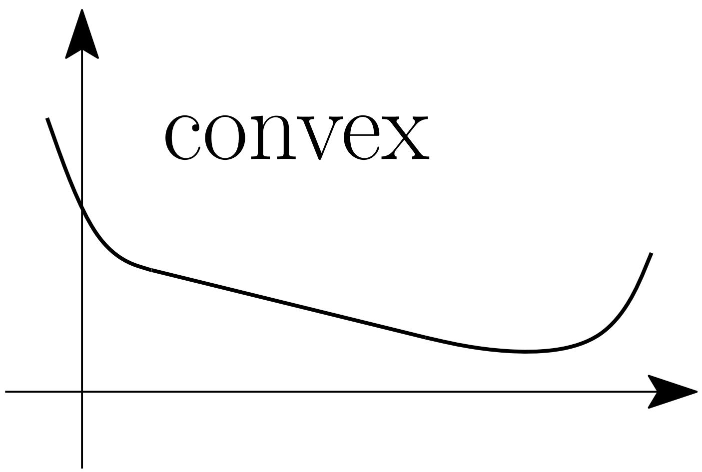

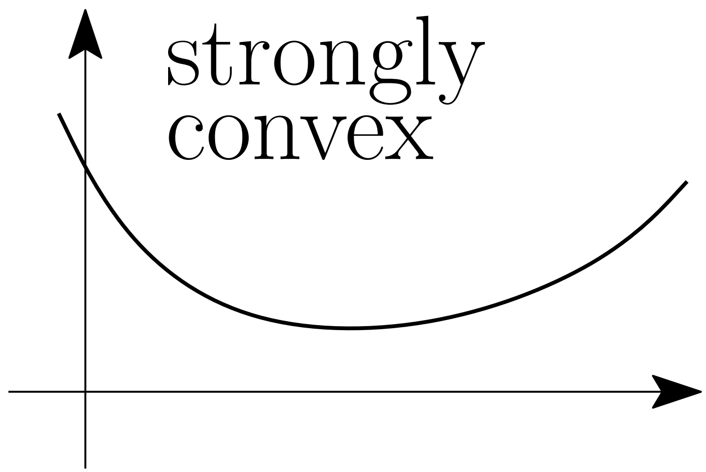

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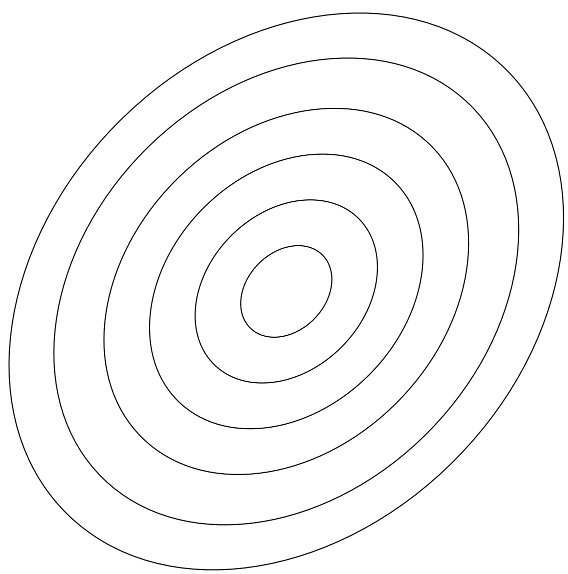
  - Condition number $\kappa = L/\mu \geqslant 1$



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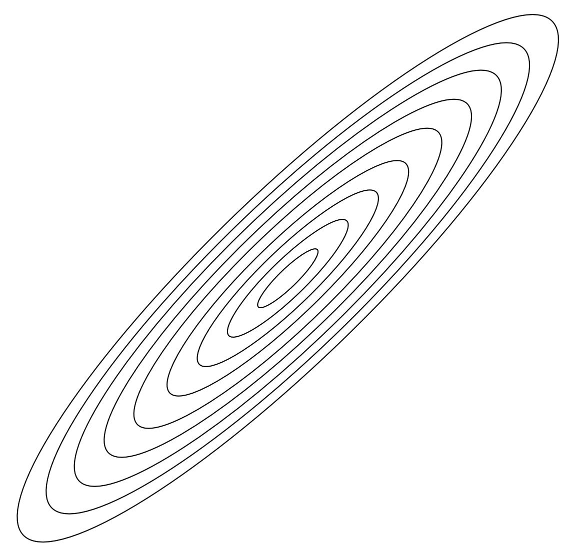

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- **Convexity in machine learning**
  - With $g(\theta) = \frac{1}{n}\sum_{i=1}^n \ell(y_i, h(x_i, \theta))$
  - Convex loss and linear predictions $h(x, \theta) = \theta^\top \Phi(x)$

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- **Relevance of convex optimization**
  - Easier design and analysis of algorithms
  - Global minimum vs. local minimum vs. stationary points
  - Gradient-based algorithms only need convexity for their analysis

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- **Strong convexity in machine learning**
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  - Invertible covariance matrix $\frac{1}{n}\sum_{i=1}^n \Phi(x_i)\Phi(x_i)^\top \Rightarrow n \geqslant d$
  - Even when $\mu > 0$, μ may be arbitrarily small!

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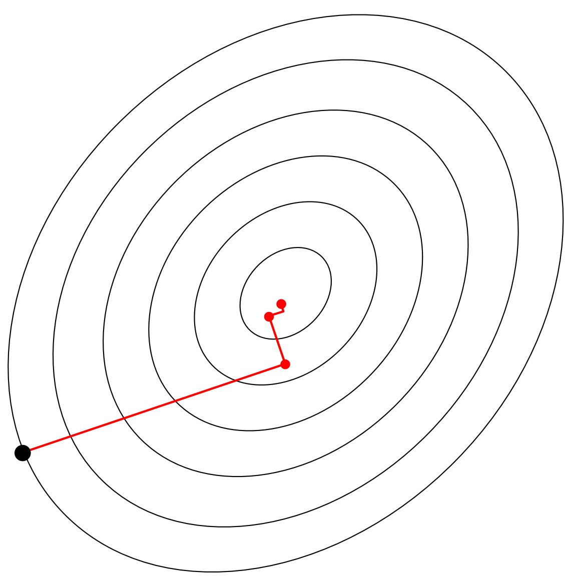
- **Adding regularization by $\frac{\mu}{2}\|\theta\|^2$**
  - creates additional bias unless μ is small, but reduces variance
  - Typically $L/\sqrt{n} \geqslant \mu \geqslant L/n \Rightarrow \kappa \in [\sqrt{n}, n]$

Iterative methods for minimizing smooth functions

- **Assumption**: g convex and L-smooth on $\mathbb{R}^d$
- **Gradient descent**: $\theta_t = \theta_{t-1} - \gamma_t \, g'(\theta_{t-1})$ *(line search)*



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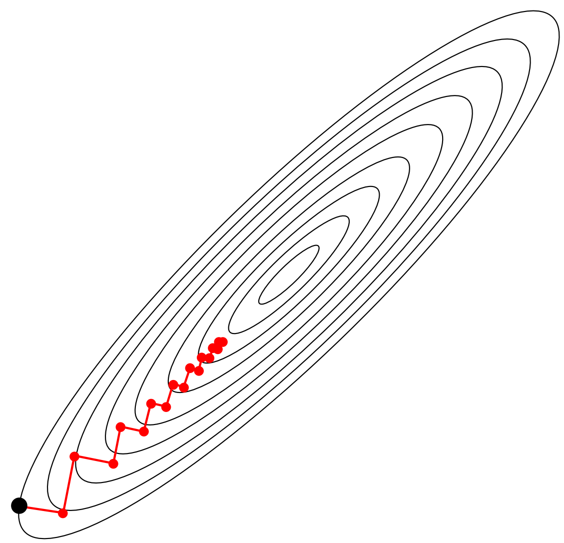

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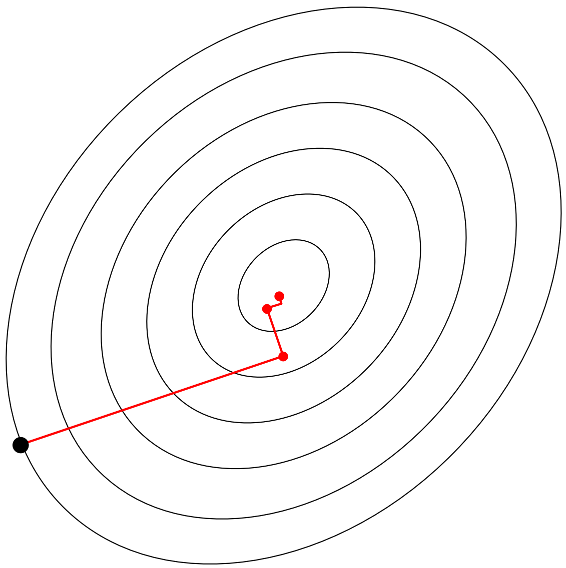

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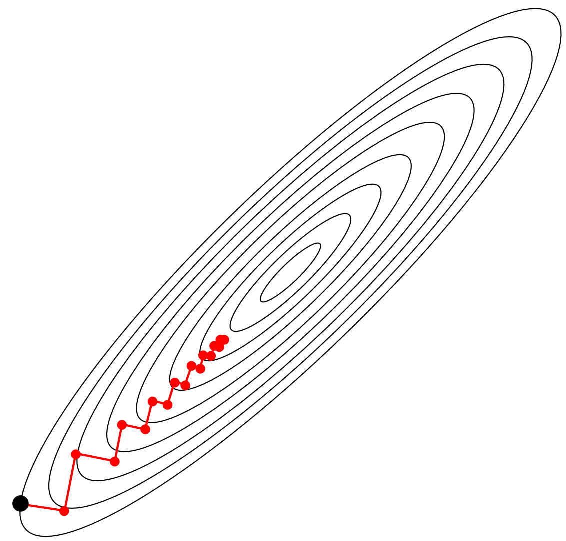

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- **Acceleration** (Nesterov, 1983): second-order recursion

$$\theta_t = \eta_{t-1} - \gamma_t g'(\eta_{t-1}) \text{ and } \eta_t = \theta_t + \delta_t(\theta_t - \theta_{t-1})$$

  – Good choice of momentum term $\delta_t \in [0, 1)$

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  - Good choice of momentum term $\delta_t \in [0,1)$
    $g(\theta_t) - g(\theta_*) \leqslant O(1/t^2)$
    $g(\theta_t) - g(\theta_*) \leqslant O((1-1/\sqrt{\kappa})^t) = O(e^{-t/\sqrt{\kappa}})$ if μ-strongly convex
  - Optimal rates after $t = O(d)$ iterations (Nesterov, 2004)

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- **Newton method**: $\theta_t = \theta_{t-1} - g''(\theta_{t-1})^{-1} g'(\theta_{t-1})$
  - $O\big(e^{-\rho 2^t}\big)$ *quadratic* rate

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- **Key insights for machine learning (Bottou and Bousquet, 2008)**
  1. No need to optimize below statistical error
  2. Cost functions are averages
  3. Testing error is more important than training error

Iterative methods for minimizing smooth functions

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

- **Gradient descent**: $\theta_t = \theta_{t-1} - \gamma_t \, g'(\theta_{t-1})$
  - $O(1/t)$ convergence rate for convex functions
  - $O(e^{-t/\kappa})$ *linear* if strongly-convex $\Leftrightarrow$ complexity $= O(nd \cdot \kappa \log \frac{1}{\varepsilon})$

- **Newton method**: $\theta_t = \theta_{t-1} - g''(\theta_{t-1})^{-1} g'(\theta_{t-1})$
  - $O\big(e^{-\rho 2^t}\big)$ *quadratic* rate $\Leftrightarrow$ complexity $= O((nd^2 + d^3) \cdot \log \log \frac{1}{\varepsilon})$

- **Key insights for machine learning (Bottou and Bousquet, 2008)**
  1. No need to optimize below statistical error
  2. Cost functions are averages
  3. Testing error is more important than training error

Stochastic gradient descent (SGD) for finite sums

$$\min_{\theta\in\mathbb{R}^d} g(\theta) = \frac{1}{n}\sum_{i=1}^{n} f_i(\theta)$$

- **Iteration**: $\theta_t = \theta_{t-1} - \gamma_t f'_{i(t)}(\theta_{t-1})$
  - Sampling with replacement: $i(t)$ random element of $\{1,\dots,n\}$
  - Polyak-Ruppert averaging: $\bar\theta_t = \frac{1}{t+1}\sum_{u=0}^{t}\theta_u$

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- **Convergence rate** if each f_i is convex L-smooth and g μ-strongly-convex:

$$\mathbb{E} g(\bar{\theta}_t) - g(\theta_*) \leqslant \begin{cases} O(1/\sqrt{t}) & \text{if } \gamma_t = 1/(L\sqrt{t}) \\ O(L/(\mu t)) = O(\kappa/t) & \text{if } \gamma_t = 1/(\mu t) \end{cases}$$

  - No adaptivity to strong-convexity in general
  - Running-time complexity: $O(d \cdot \kappa/\varepsilon)$

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- **NB**: single pass leads to bounds on testing error

Stochastic vs. deterministic methods

- Minimizing $g(\theta) = \frac{1}{n}\sum_{i=1}^{n} f_i(\theta)$ with $f_i(\theta) = \ell\big(y_i, h(x_i, \theta)\big) + \lambda\Omega(\theta)$

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  - Can be accelerated to $O(e^{-t/\sqrt{\kappa}})$ (Nesterov, 1983)
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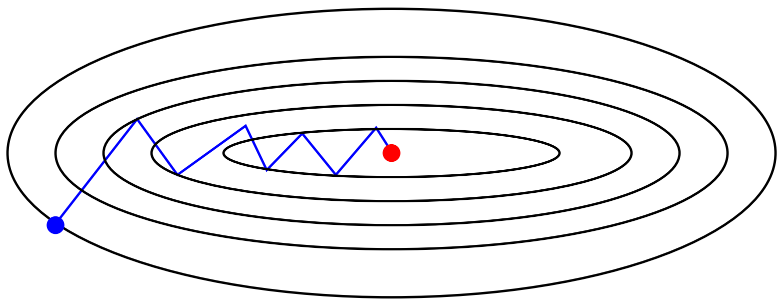

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  - Iteration complexity is independent of n

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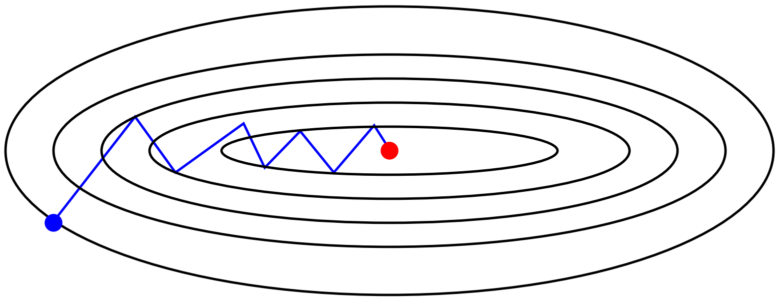

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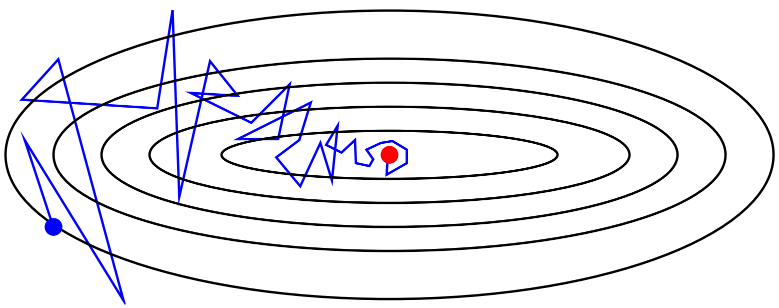
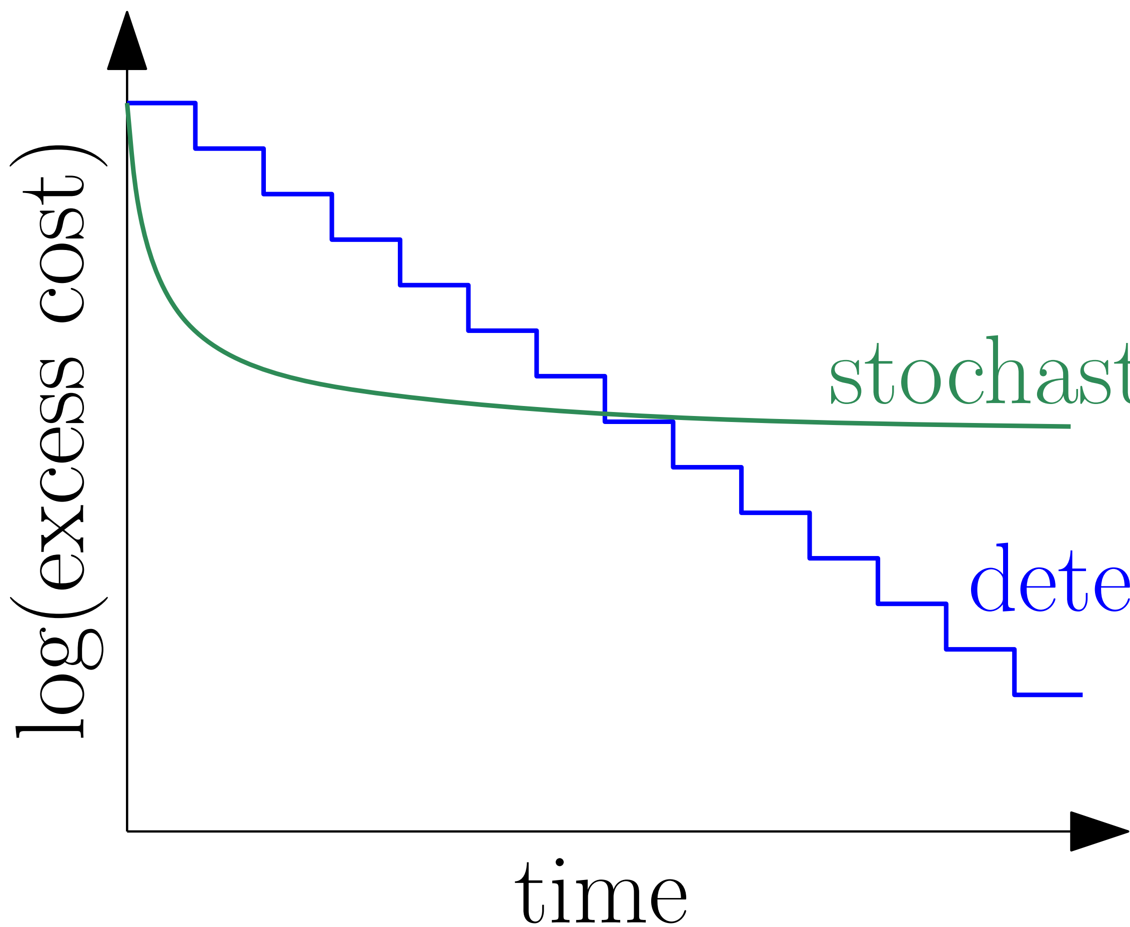


Stochastic vs. deterministic methods

- **Goal = best of both worlds**: Linear rate with $O(d)$ iteration cost
  Simple choice of step size



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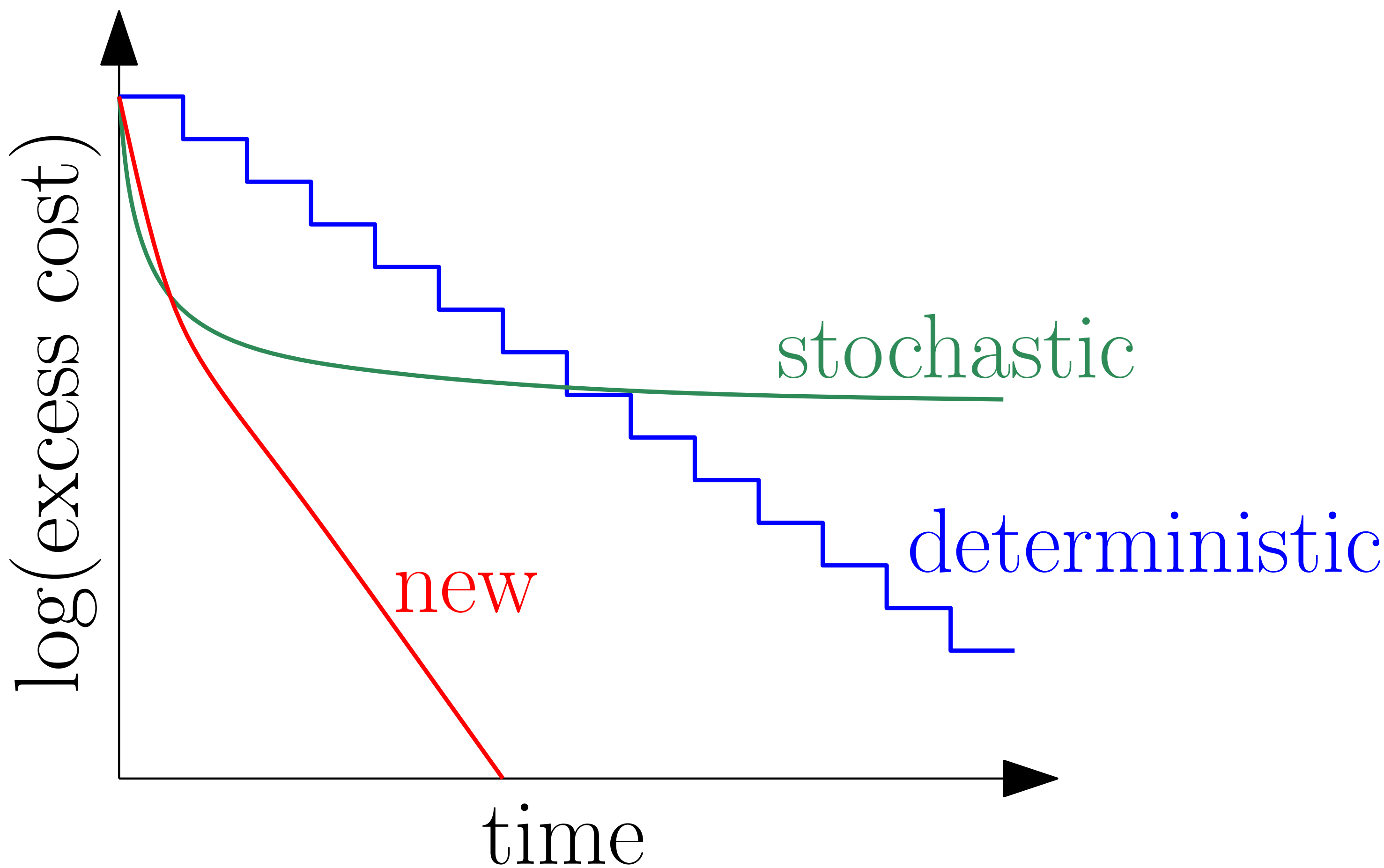

Recent progress in single machine optimization

- **Variance reduction**
  - Exponential convergence with $O(d)$ iteration cost
  - SAG (Le Roux, Schmidt, and Bach, 2012)
  - SVRG (Johnson and Zhang, 2013; Zhang et al., 2013)
  - SAGA (Defazio, Bach, and Lacoste-Julien, 2014), etc...

$$\theta_t = \theta_{t-1} - \gamma \Big[\nabla f_{i(t)}(\theta_{t-1}) \qquad\qquad\qquad\qquad \Big]$$

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$$\theta_t = \theta_{t-1} - \gamma\Big[\nabla f_{i(t)}(\theta_{t-1}) + \frac{1}{n}\sum_{i=1}^{n} y_i^{t-1} - y_{i(t)}^{t-1}\Big]$$

(with y_i^t stored value at time t of gradient of the i-th function)

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- **Running-time to reach precision** ε (with $\kappa =$ condition number)

Stochastic gradient descent	$d\times$	κ	$\times$	$\frac{1}{\varepsilon}$
Gradient descent	$d\times$	$n\kappa$	$\times \log$	$\frac{1}{\varepsilon}$
Variance reduction	$d\times$	$(n+\kappa)$	$\times \log$	$\frac{1}{\varepsilon}$

  - Can be accelerated (e.g., Lan, 2015): $n+\kappa \Rightarrow n+\sqrt{n\kappa}$
  - Matching upper and lower bounds of complexity

Outline

1. **Parametric supervised learning on a single machine**
   - Machine learning $\approx$ optimization of finite sums
   - From batch to stochastic gradient methods
   - Linearly-convergent stochastic methods for convex problems

2. **Machine learning over networks**
   - Centralized and decentralized methods
   - From network averaging to optimization
   - Distributing the fastest single machine algorithms

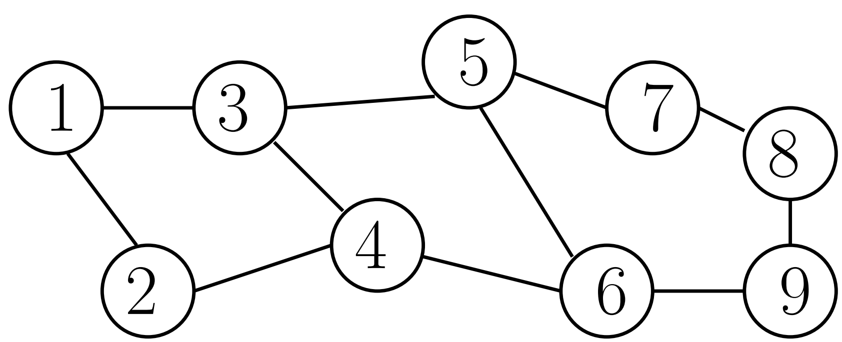
Distribution in machine learning (and beyond)

- **Machine learning through optimization**

$$\min_{\theta \in \mathbb{R}^d} \quad \frac{1}{n} \sum_{i=1}^{n} f_i(\theta) = g(\theta)$$

  - $f_i(\theta)$ error of model defined by θ on dataset indexed by i

- **Each dataset / function f_i only accessible by node i in a graph**



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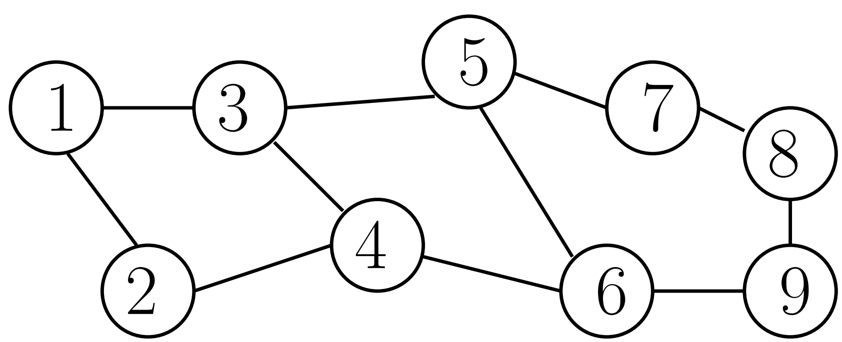

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- **Each dataset / function f_i only accessible by node i in a graph**
  - Massive datasets, multiple machines / cores
  - Communication / legal constraints

- **Goal: Minimize communication and local computation costs**

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- **Why not simply distributing a simple single machine algorithm?**

  – (accelerated) gradient descent (see, e.g., Nesterov, 2004)

$$\theta_t = \theta_{t-1} - \gamma \nabla g(\theta_{t-1})$$

  – Requires $\sqrt{\kappa} \log \frac{1}{\varepsilon}$ full gradient computations to reach precision ε

  – Need to perform distributed averaging over a network

Classical algorithms for distributed averaging

- **Goal**: Given n observations $\xi_1, \dots, \xi_n \in \mathbb{R}$
  - Compute $\theta_* = \dfrac{1}{n}\sum_{i=1}^{n} \xi_i = \arg\min_{\theta \in \mathbb{R}} \ \dfrac{1}{n}\sum_{i=1}^{n}(\theta - \xi_i)^2$

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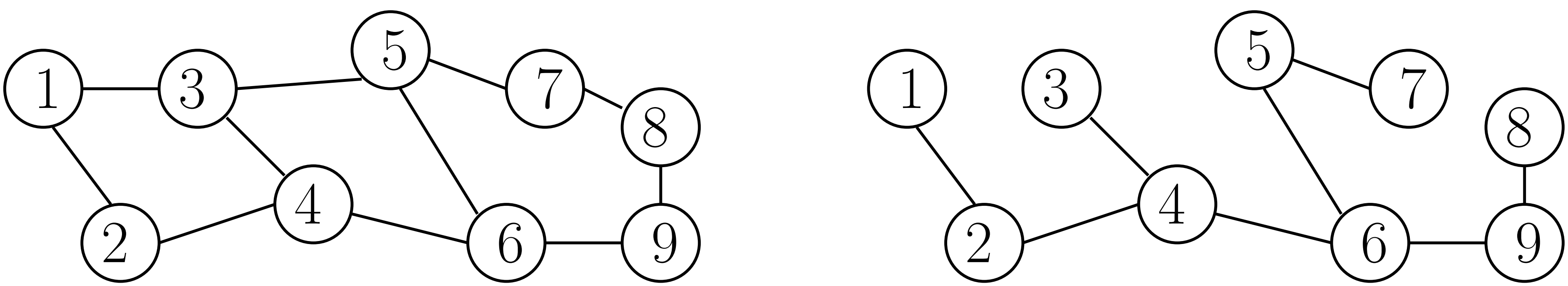
- **Centralized algorithms**
  - Compute a spanning tree with diameter $\leqslant 2\Delta$
  - Master/slave algorithm



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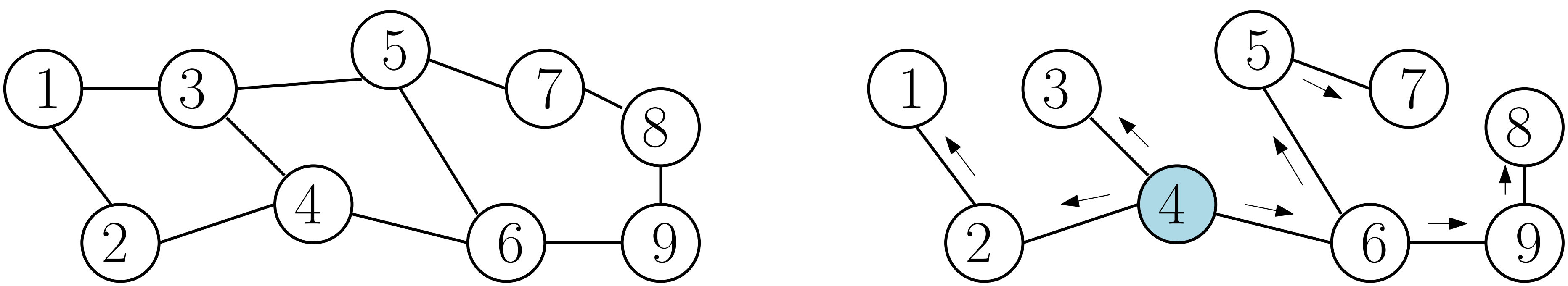

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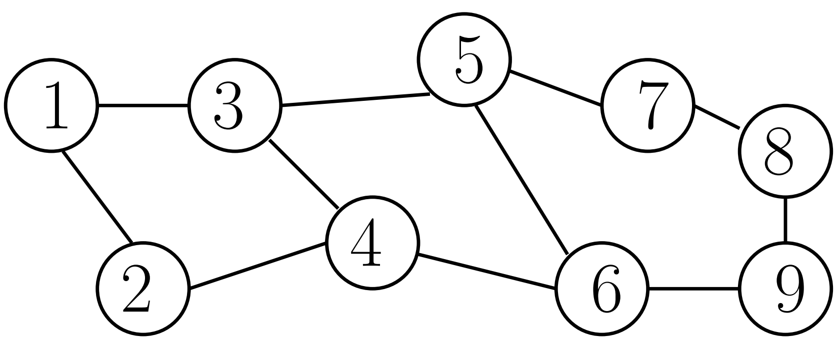

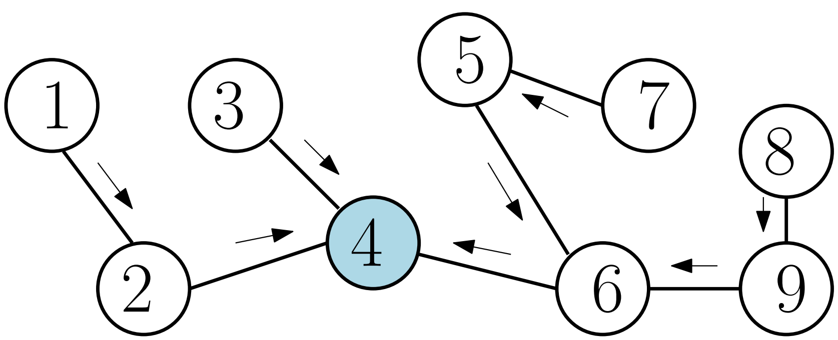

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  - $\sqrt{\kappa}\log\frac{1}{\varepsilon}$ gradient steps and $\sqrt{\kappa}\Delta\log\frac{1}{\varepsilon}$ communication steps
  - "Optimal" (Scaman, Bach, Bubeck, Lee, and Massoulié, 2017)

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- **Robustness?**

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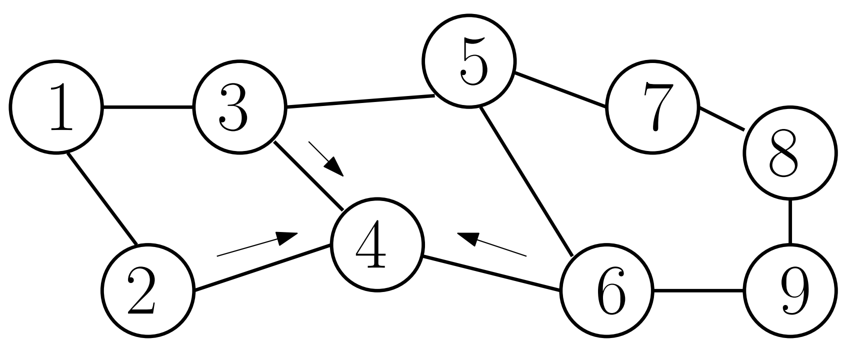
  - Replace θ_i by a weighted average of its neighbors $\sum_{j=1}^n W_{ij}\theta_j$



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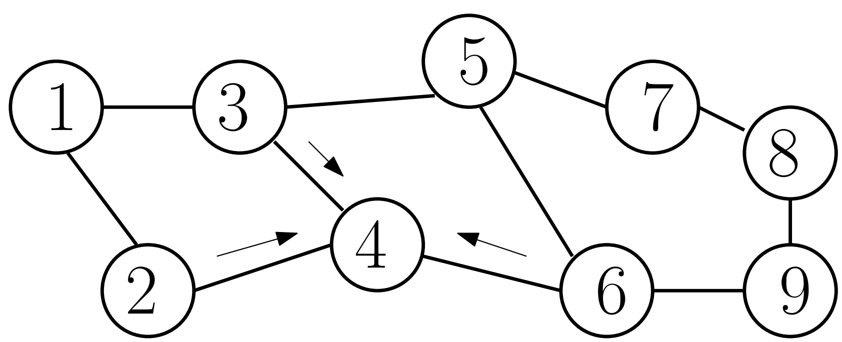

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- **Synchronous gossip** (all nodes simultaneously)
  - Main iteration: $\boxed{\theta_t = W\theta_{t-1} = W^t\theta_0 = W^t\xi}$
  - Typical assumption: W symmetric doubly stochastic matrix

Convergence of synchronous gossip

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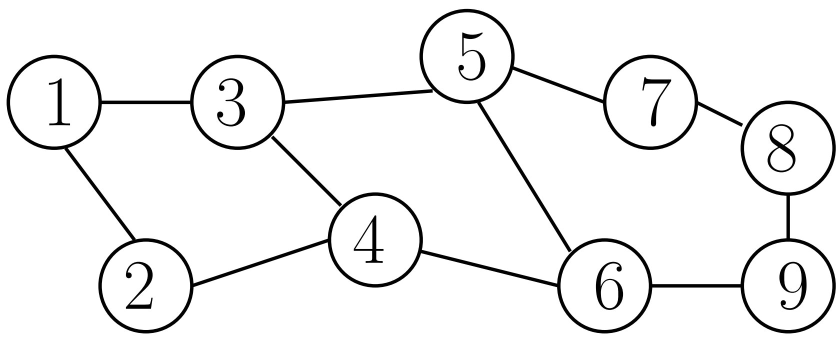
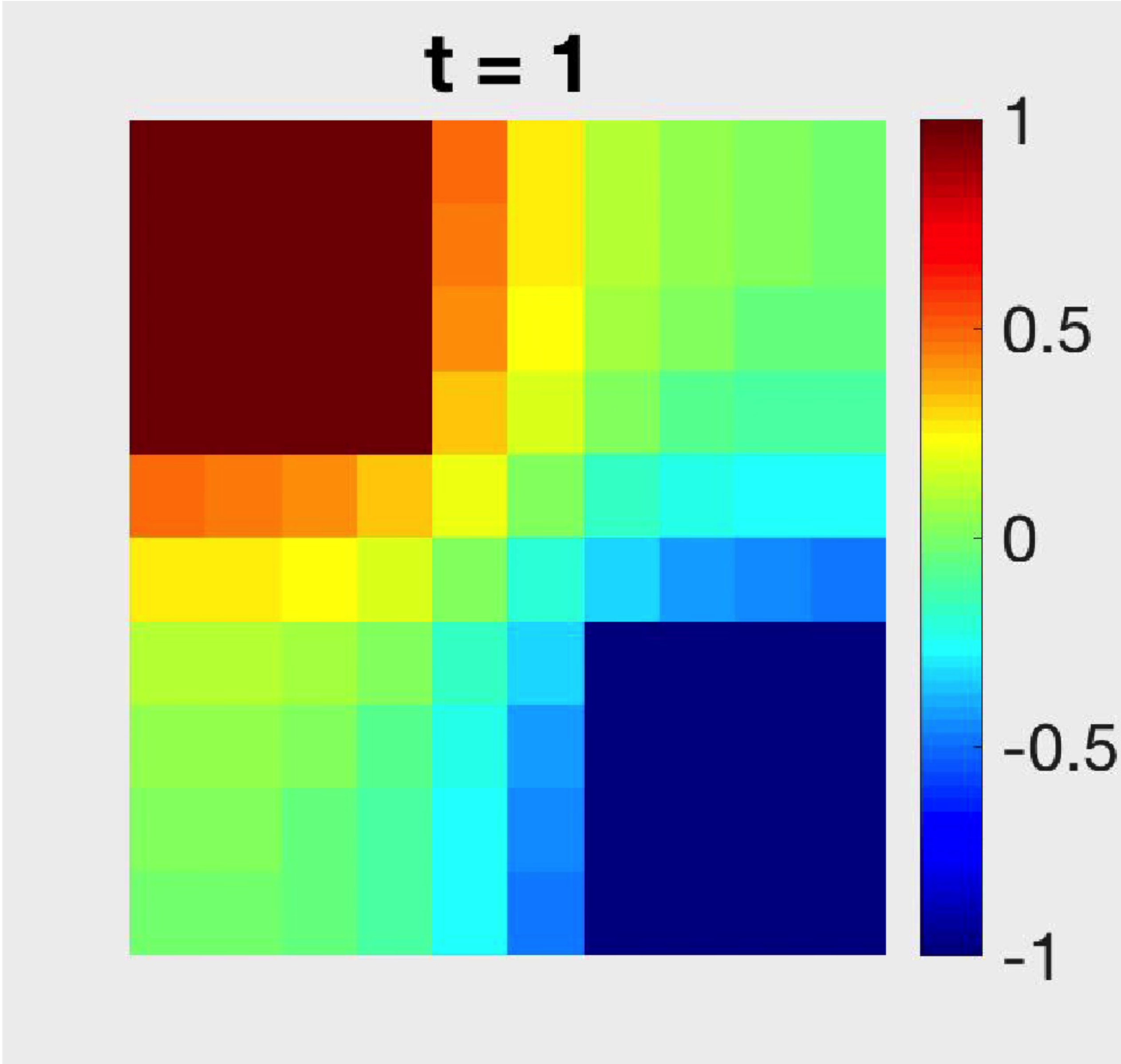
  - Typical assumption: W symmetric doubly stochastic matrix
  - Consequence: Eigenvalues$(W) \in [-1, 1]$
  - Eigengap $\gamma = \lambda_1(W) - \lambda_2(W) = 1 - \lambda_2(W)$
  - γ^{-1} = mixing time of the associated Markov chain



  - Need $\frac{1}{\gamma}\log\frac{1}{\varepsilon}$ iterations to reach precision ε (for classical averaging)

Illustration of synchronous gossip



Decentralized optimization

- **Mixing gossip and optimization**
  - Nedic and Ozdaglar (2009); Duchi et al. (2012); Wei and Ozdaglar (2012); Iutzeler et al. (2013); Shi et al. (2015); Jakovetić et al. (2015); Nedich et al. (2016); Mokhtari et al. (2016); Colin et al. (2016); Scaman et al. (2017), **etc.**

Decentralized optimization

- **Mixing gossip and optimization**

- **Lower bound on complexity** (Scaman et al., 2017)
  - $\sqrt{\kappa} \log \frac{1}{\varepsilon}$ gradient steps and $\sqrt{\kappa/\gamma} \log \frac{1}{\varepsilon}$ communication steps
  - Plain gossip not optimal!
    (need to gossip gradients with increasing precision)

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  - $\sqrt{\kappa}\log\frac{1}{\varepsilon}$ gradient steps and $\sqrt{\kappa/\gamma}\log\frac{1}{\varepsilon}$ communication steps
  - Plain gossip not optimal!
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- **Is this lower bound achievable?**

Dual reformulation (Jakovetić et al., 2015)

$$\min_{\theta \in \mathbb{R}^d} \sum_{i=1}^{n} f_i(\theta) = \min_{\theta^{(1)},\ldots,\theta^{(n)} \in \mathbb{R}^d} \sum_{i=1}^{n} f_i(\theta^{(i)}) \text{ such that } \forall i \sim j, \theta^{(i)} = \theta^{(j)}$$

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$$= \max_{\forall i\sim j, \lambda_{ij}\in\mathbb{R}^d}\ \min_{\theta^{(1)},\dots,\theta^{(n)}\in\mathbb{R}^d}\sum_{i=1}^n f_i(\theta^{(i)}) + \sum_{i=1}^n[\theta^{(i)}]^\top \text{linear}_i(\lambda)$$

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$$= \min_{\theta^{(1)},\dots,\theta^{(n)}\in\mathbb{R}^d} \max_{\forall i\sim j, \lambda_{ij}\in\mathbb{R}^d} \sum_{i=1}^n f_i(\theta^{(i)}) + \sum_{i\sim j} \lambda_{ij}^\top(\theta^{(i)} - \theta^{(j)})$$

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$$= \max_{\forall i\sim j, \lambda_{ij}\in\mathbb{R}^d} \sum_{i=1}^n \text{function}_i(\lambda) = \max_{\forall i\sim j, \lambda_{ij}\in\mathbb{R}^d} \text{function}(\lambda)$$

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$$\min_{\theta\in\mathbb{R}^d}\sum_{i=1}^n f_i(\theta) = \min_{\theta^{(1)},\dots,\theta^{(n)}\in\mathbb{R}^d}\sum_{i=1}^n f_i(\theta^{(i)}) \text{ such that } \forall i\sim j, \theta^{(i)}=\theta^{(j)}$$

$$= \min_{\theta^{(1)},\dots,\theta^{(n)}\in\mathbb{R}^d}\ \max_{\forall i\sim j,\lambda_{ij}\in\mathbb{R}^d}\sum_{i=1}^n f_i(\theta^{(i)}) + \sum_{i\sim j}\lambda_{ij}^\top(\theta^{(i)}-\theta^{(j)})$$

$$= \max_{\forall i\sim j,\lambda_{ij}\in\mathbb{R}^d}\ \min_{\theta^{(1)},\dots,\theta^{(n)}\in\mathbb{R}^d}\sum_{i=1}^n f_i(\theta^{(i)}) + \sum_{i=1}^n[\theta^{(i)}]^\top \text{linear}_i(\lambda)$$

$$= \max_{\forall i\sim j,\lambda_{ij}\in\mathbb{R}^d}\sum_{i=1}^n \text{function}_i(\lambda) = \max_{\forall i\sim j,\lambda_{ij}\in\mathbb{R}^d}\text{function}(\lambda)$$

- **Accelerated gradient descent** (Scaman et al., 2017)
  $\Leftrightarrow$ alternating local gradient computations and a gossip step
  - $\sqrt{\kappa/\gamma}\log\frac{1}{\varepsilon}$ gradient steps and $\sqrt{\kappa/\gamma}\log\frac{1}{\varepsilon}$ communication steps
  - Not optimal $\Rightarrow$ need accelerated gossip

Accelerated gossip

- **Regular gossip**
  - Iterations: $\theta_t = W^t \theta_0$

- **Accelerated gossip**
  - Chebyshev acceleration (Auzinger, 2011; Arioli and Scott, 2014)
  - Shift-register gossip (Cao et al., 2006)
  - Linear combinations $\Leftrightarrow \eta_t = \sum_{k=0}^{t} \alpha_k \theta_k = \sum_{k=0}^{t} \alpha_k W^k \xi = P_t(W)\xi$
  - Optimal polynomial is the Chebyshev polynomial
  - Can be computed online with same cost as regular gossip, e.g.,

$$\theta_t = \omega_t W \theta_{t-1} + (1 - \omega_t)\theta_{t-1}$$

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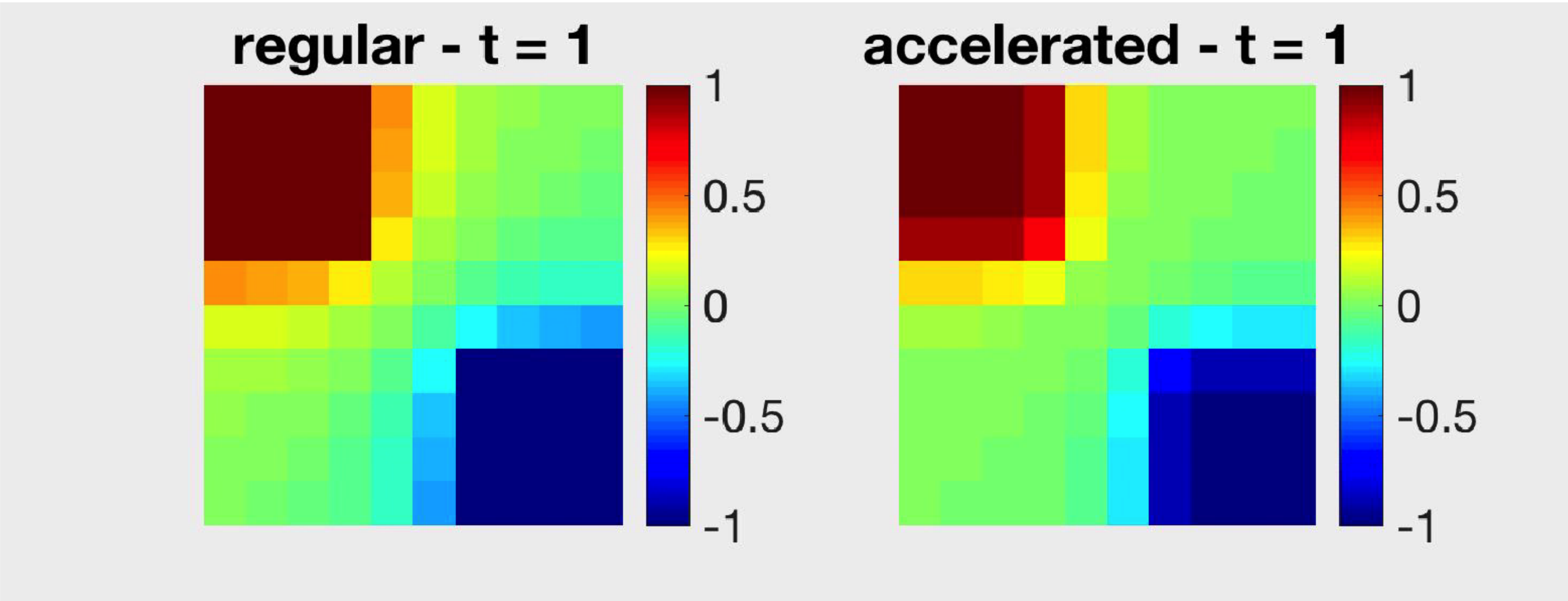
  - Replace γ^{-1} by $\gamma^{-1/2}$ in rates

Illustration of accelerated gossip



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- $\Rightarrow$ **optimal complexity for optimization** (Scaman et al., 2017)

Distribution in machine learning (and beyond)

- **Machine learning through optimization**

$$\min_{\theta \in \mathbb{R}^d} \quad \frac{1}{n} \sum_{i=1}^{n} f_i(\theta) = g(\theta)$$

  – $f_i(\theta)$ error of model defined by θ on dataset indexed by i

  – Example: $f_i(\theta) = \dfrac{1}{m_i} \sum_{j=1}^{m_i} \ell(y_{ij}, \theta^\top \Phi(x_{ij}))$ if m_i observations

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- **Single machine vs. "optimal" decentralized algorithm**

Algorithm	gradient steps	communication
Single machine algorithm	$nm + \sqrt{nm\kappa}$	0
MSDA (Scaman et al., 2017)	$m\sqrt{\kappa}$	$\sqrt{\kappa/\gamma}$

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- **MSDA (Scaman et al., 2017)**
  - $\sqrt{\kappa} \log \frac{1}{\varepsilon}$ gradient steps and $\sqrt{\kappa/\gamma} \log \frac{1}{\varepsilon}$ communication steps
  - "Optimal", but still not adapted to machine learning
  - Huge slow down when going from 1 to 2 machines
  - Only synchronous

Decentralized algorithms for machine learning (Hendrikx, Bach, and Massoulié, 2019)

- **Trade-offs between gradient and communication steps**
  - Adapted to functions of the type $f_i(\theta) = \frac{1}{m}\sum_{j=1}^{m} \ell(y_{ij}, \theta^\top \Phi(x_{ij}))$
  - Allows for partial asynchrony
- n **computing nodes, with** m **observations each**

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Single machine algorithm	$nm + \sqrt{nm\kappa}$	0
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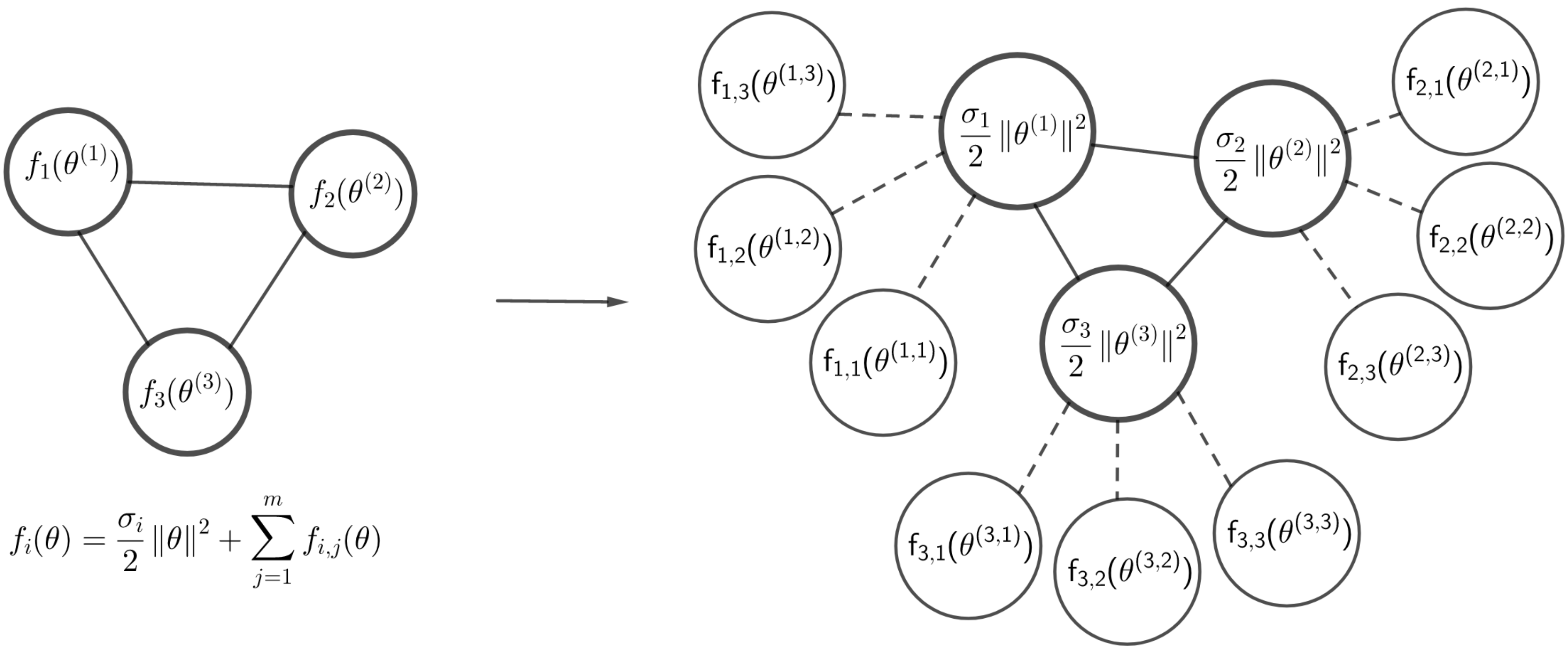
ADFS (Hendrikx et al., 2019)	$m + \sqrt{m\kappa}$	$\sqrt{\kappa/\gamma}$

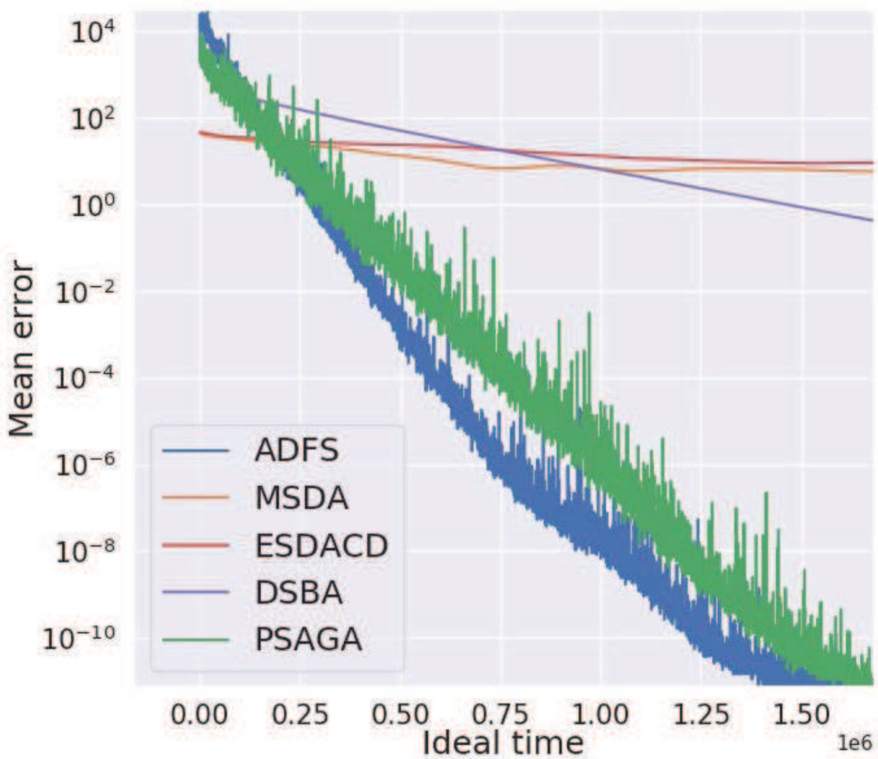
ADFS - Algorithm principle

- **Minimizing** $\sum_{i=1}^{n} \Big\{ \sum_{j=1}^{m} f_{i,j}(\theta) + \frac{\sigma_i}{2} \|\theta\|^2 \Big\}$
  - Create an equivalent graph
  - Dual randomized coordinate ascent (with non uniform sampling)
  - Decoupling of data and gossip steps

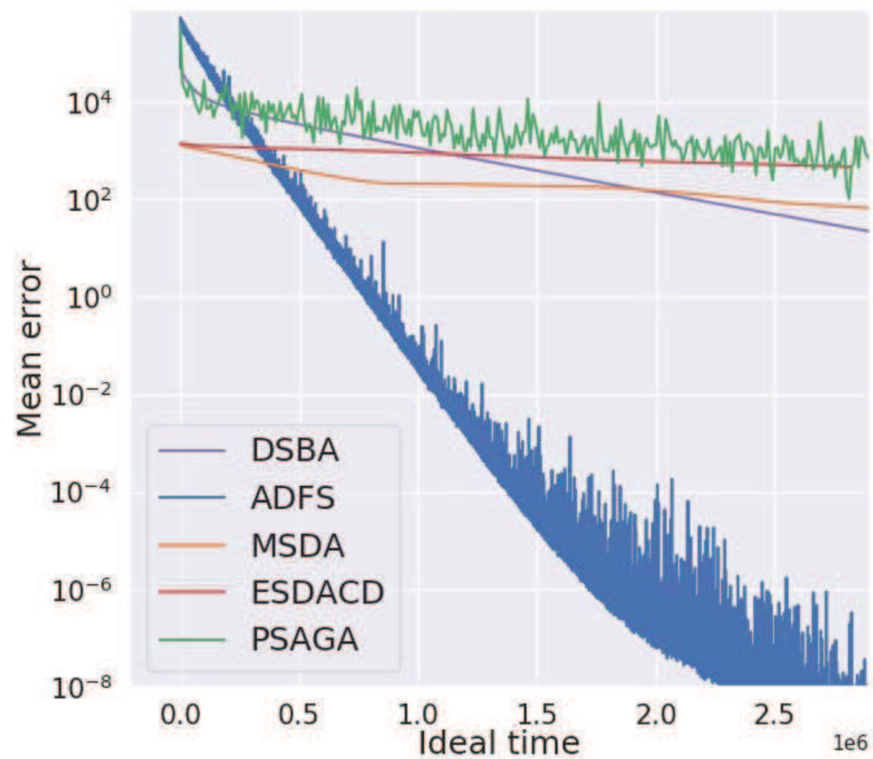


Decentralized algorithms for machine learning (Hendrikx, Bach, and Massoulié, 2019)

- **Running times on an actual cluster**
  - Logistic regression with $m = 10^4$ observations per node in $\mathbb{R}^{28}$
  - Two-dimensional grid network



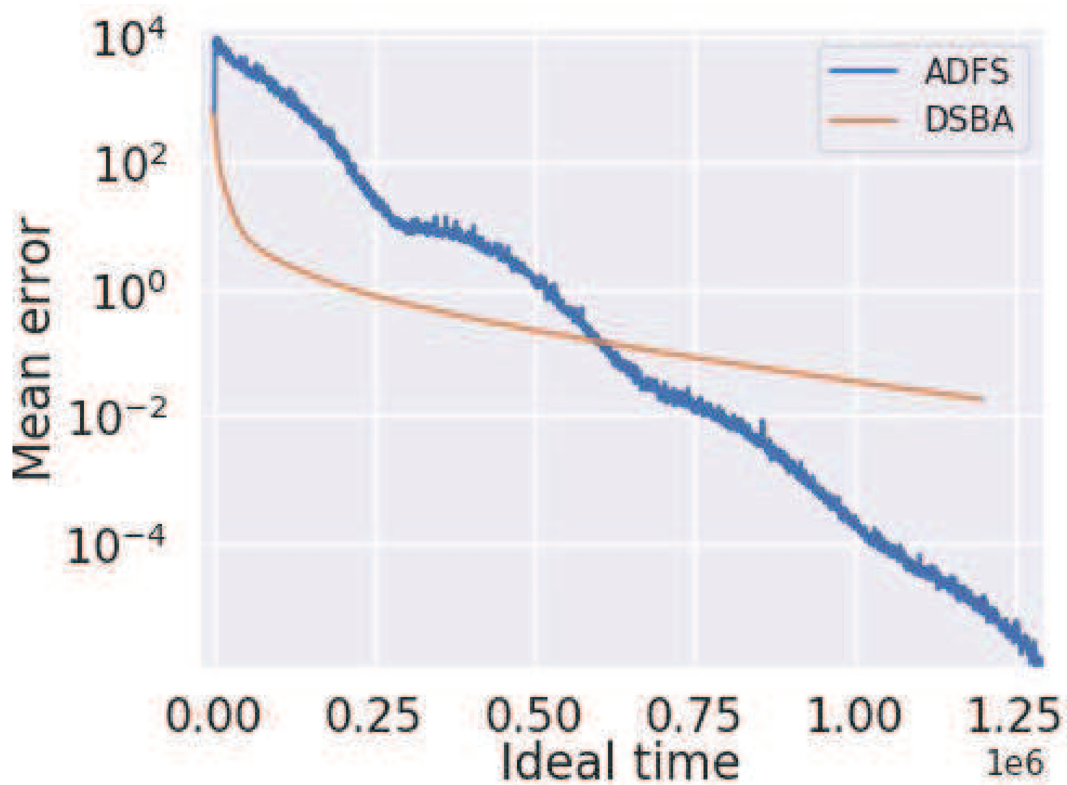
$n = 4$



$n = 100$

Decentralized algorithms for machine learning (Hendrikx, Bach, and Massoulié, 2019)

- **Running times on an actual cluster**
  - Logistic regression with $mn \approx 10^5$ observations in $\mathbb{R}^{47236}$
  - Two-dimensional grid network with $n = 100$ nodes



Conclusions

- **Distributed decentralized machine learning**
  - Distributing the fastest single machine algorithms!
  - n machines and m observations per machine
  - From $nm + \sqrt{nm\kappa}$ (single machine) to $m + \sqrt{m\kappa}$ gradient steps
  - Linear speed-ups for well-conditioned problems

Conclusions

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  - From $nm + \sqrt{nm\kappa}$ (single machine) to $m + \sqrt{m\kappa}$ gradient steps
  - Linear speed-ups for well-conditioned problems
- **Extensions**
  - Beyond convex problems
  - Matching running time complexity lower bounds
  - Experiments on large-scale clouds

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