Tracking the gradients using the Hessian: A new look at variance reducing stochastic methods

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Joint work with Nicolas Le Roux and Francis Bach

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Solve Empirical Risk Minimization

$$\min_{\theta \in \mathbf{R}^d} f(\theta) \stackrel{\text{def}}{=} \frac{1}{n} \sum_{i=1}^{n} f_i(\theta),$$

where n is the num of data points and $d$the num of features.

Datum functions	$f_i(\theta)$ is twice differentiable
Ridge Regression	$f_i(\theta) = (y^i - \langle \theta, x^i \rangle)^2 + \lambda \|\|\theta\|\|_2^2$
Logistic regression	$f_i(\theta) = \ln(1 + e^{-y^i \langle \theta, x^i \rangle}) + \lambda \|\|\theta\|\|_2^2$
Some neural nets	$f_i(\theta) = \dots$

Using a first order gradient method

$$\theta_{t+1} = \theta_t - \gamma g_t$$

Stepsize $\gamma > 0$

Unbiased

$$\mathbb{E}[g_t] = \nabla f(\theta_t)$$

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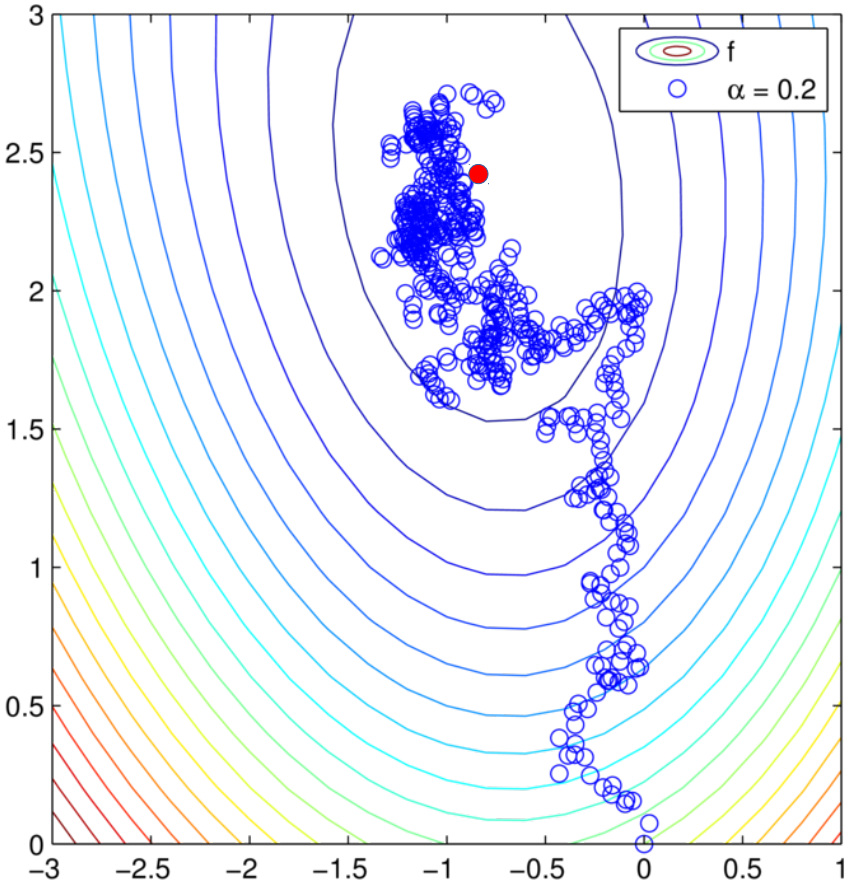
EXE: Stochastic Gradient descent (SGD)

$$g_t = \nabla f_i(\theta_t), \quad \text{where } i \sim \mathcal{U}\{1, \ldots, n\}$$

Stochastic Gradient Descent γ = 0.2



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EXE: SGD with covariates

$$g_t = \nabla f_i(\theta_t) - z_i + \frac{1}{n}\sum_{j=1}^{n} z_j, \text{ where } i \sim \mathcal{U}\{1, \ldots, n\}$$

$$z_i \in \mathbb{R}^d, \text{ for } i = 1, \ldots, n$$

Choosing the covariates

SGD with covariates:

$$g_t = \nabla f_i(\theta_t) - z_i + \frac{1}{n}\sum_{j=1}^{n} z_j$$

1) Correlated to the stochastic gradients

$$\text{If } \nabla f_i(\theta_t) \approx z_i \text{ then } \mathbb{VAR}(g_t) \leq \mathbb{VAR}(\nabla f_i(\theta_t))$$

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$$\text{cost}(g_t) \quad \leq \quad \text{cost}\big(\frac{1}{n}\sum_{j=1}^{n} \nabla f_j(\theta_t)\big)$$

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EXE: Too costly

$$z_i = \nabla f_i(\theta_t)$$

$$g_t = \nabla f(\theta_t)$$

EXE: High variance

$$z_i = 0$$

$$g_t = \nabla f_i(\theta_t)$$

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EXE: Too costly

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$$g_t = \nabla f(\theta_t)$$

Want something in between

EXE: High variance

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$$g_t = \nabla f_i(\theta_t)$$

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$$\theta_{t+1} = \theta_t - \gamma g_t$$

Reference point $\tilde{\theta} \in \mathbb{R}^d$

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Set $\theta_0 = 0$, choose $\gamma > 0, m \in \mathbb{N}$
$\tilde{\theta}_0 = \theta_0$
for $k = 0, 1, 2, \ldots, T-1$
    calculate $\nabla f(\tilde{\theta}_k)$
    $\theta_0 = \tilde{\theta}_k$
    for $t = 0, 1, 2, \ldots, m-1$
        sample $i \in \{1, \ldots, n\}$
        $g_t = \nabla f_i(\theta_t) - \nabla f_i(\tilde{\theta}_k) + \nabla f(\tilde{\theta}_k)$
        $\theta_{t+1} = \theta_t - \gamma g_t$
    $\tilde{\theta}_{k+1} = \theta_m$
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Johnson, R. & Zhang, T. Accelerating stochastic gradient descent using predictive variance reduction Advances in Neural Information Processing Systems, 2013, 315-323

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Freeze reference point for m iterations

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Why not 1st Taylor?

Johnson, R. & Zhang, T. Accelerating stochastic gradient descent using predictive variance reduction Advances in Neural Information Processing Systems, 2013, 315-323

SVRG2: Second order tracking

$$\theta_{t+1} = \theta_t - \gamma g_t$$

Reference point

$$\tilde{\theta} \in \mathbb{R}^d$$

1st order Taylor exp.

$$\nabla f_i(\theta_t) \approx \nabla f_i(\tilde{\theta}) + H_i(\tilde{\theta})(\theta_t - \tilde{\theta})$$

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$$H_i(\tilde{\theta}) := \nabla^2 f_i(\tilde{\theta})$$

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Expected covariate

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$$\begin{aligned} g_t &= \nabla f_i(\theta_t) - z_i + \frac{1}{n}\sum_{j=1} z_j \\ &= \nabla f_i(\theta_t) - \nabla f_i(\tilde{\theta}) + \nabla f(\tilde{\theta}) \\ &\quad + (\frac{1}{n}\sum_{j=1}^{n} H_j(\tilde{\theta}) - H_i(\tilde{\theta}))(\theta_t - \tilde{\theta}) \end{aligned}$$

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H. T. Wai, W. Shi, A. Nedic, and A. Scaglione. Curvature-aided incremental aggregated gradient method, Allerton. IEEE, 2017,

SVRG2: Stochastic Variance Reduced Gradients with tracking

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for $k = 0, 1, 2, \ldots, T-1$

calculate $\nabla f(\tilde{\theta}), \underline{H = \nabla^2 f(\tilde{\theta})}$

$\theta_0 = \tilde{\theta}$

for $t = 0, 1, 2, \ldots, m-1$

sample $i \in \{1, \ldots, n\}$

$g_t = \nabla f_i(\theta_t) - \nabla f_i(\tilde{\theta}) + \nabla f(\tilde{\theta})$

$+\underline{(H - H_i(\tilde{\theta}))(\theta_t - \tilde{\theta})}$

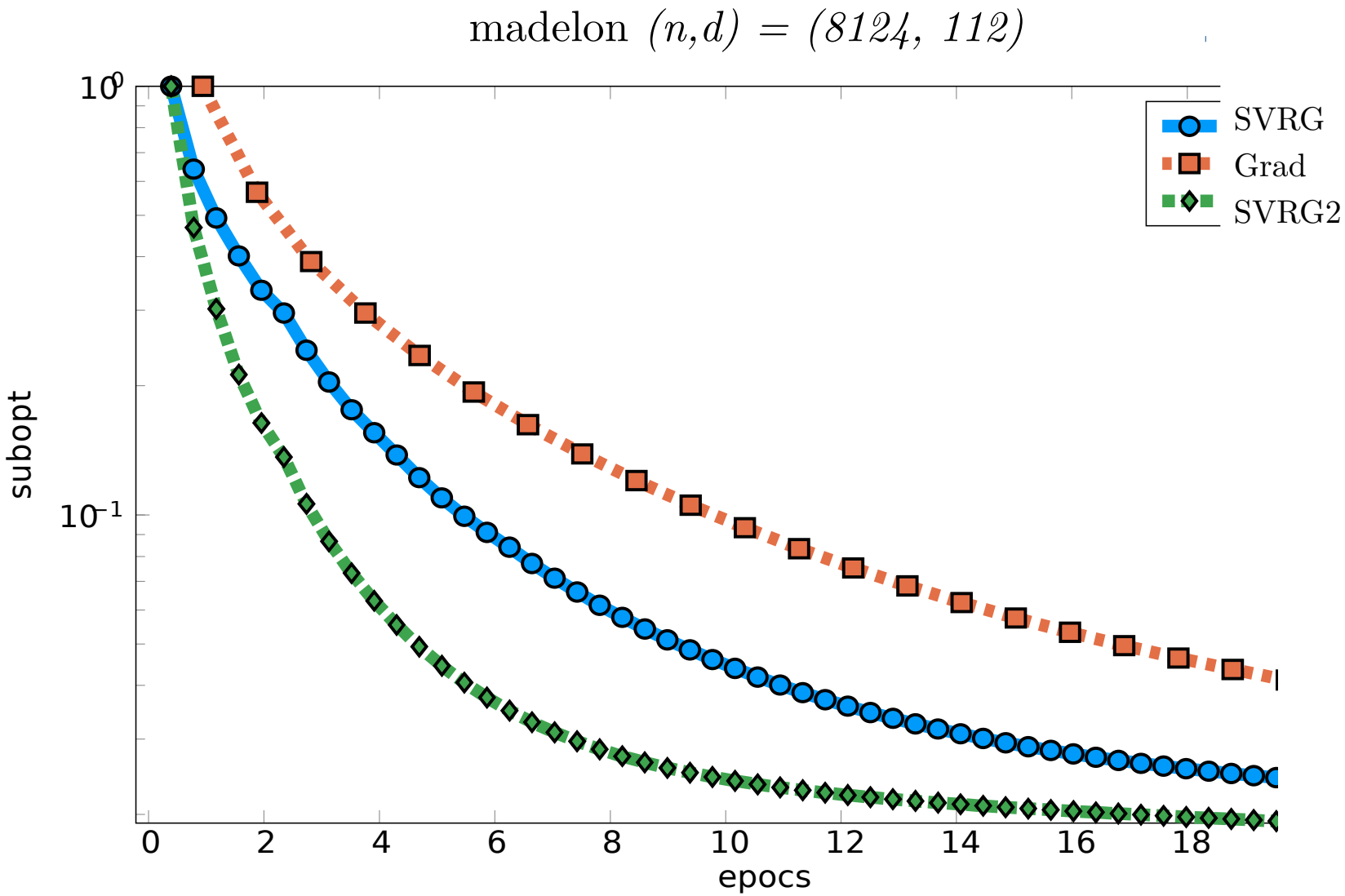
$\theta_{t+1} = \theta_t - \gamma g_t$

$\tilde{\theta} = \theta_m$

Output $\tilde{\theta}$

Does this actually work?

SVRG2: first experiment



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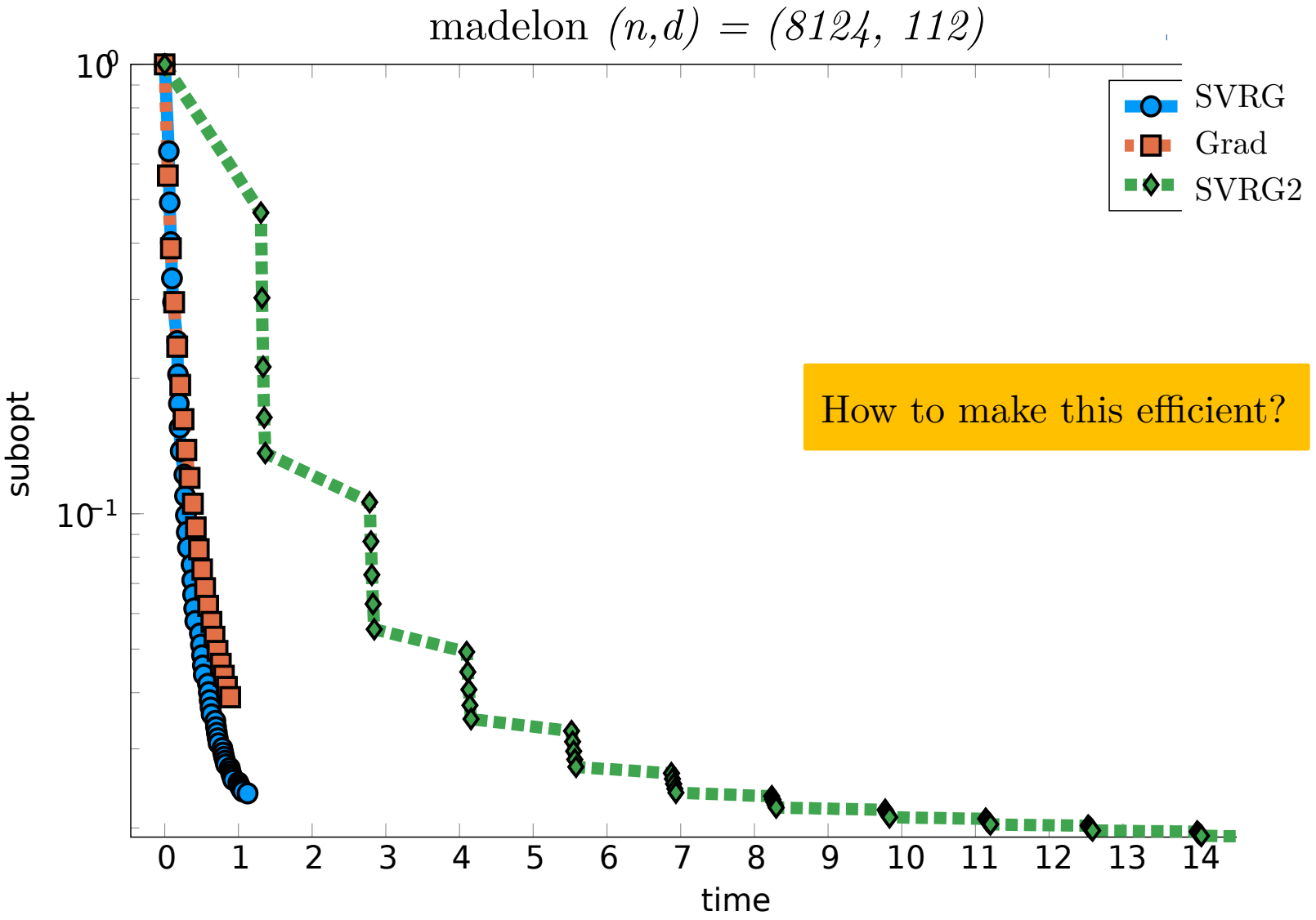

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Output $\tilde{\theta}$

Cost of SVRG2

$$g_t = \nabla f_i(\theta_t) - \nabla f_i(\tilde{\theta}) + \nabla f(\tilde{\theta}) + (\frac{1}{n}\sum_{j=1}^{n} H_j(\tilde{\theta}) - H_i(\tilde{\theta}))(\theta_t - \tilde{\theta})$$

- Full Hessian $H = \frac{1}{n}\sum_{j=1}^{n} H_j(\tilde{\theta})$ costs $O(nd \times \text{eval}(f_i))$
- Hessian vector product $H(\theta_t - \tilde{\theta})$ costs $O(d^2)$
- Directional derivative $H_i(\tilde{\theta})(\theta_t - \tilde{\theta})$ costs $O(\text{eval}(f_i))$

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Build approximations $\hat{H}_j(\theta) \approx H_j(\theta)$

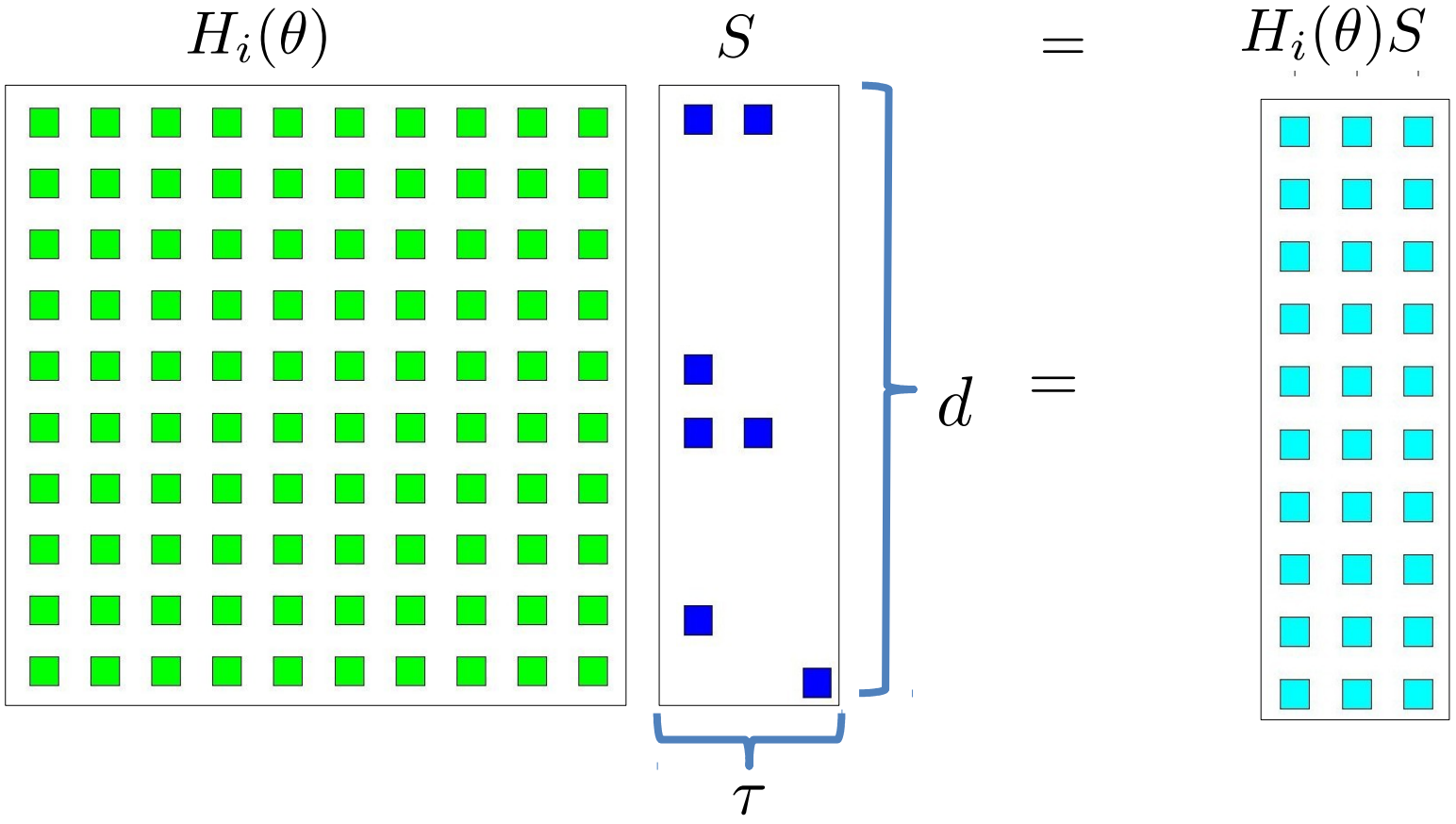
Different ways to approximate the Hessian

$$\hat{H}_i(\theta) \approx H_i(\theta)$$

We tried:

- Diagonal approximations
- Rank-1 approximation based on secant equation
- **Low rank approximations using Sketching and projecting**

Sketching the stochastic Hessian



Sketching matrix

$S \sim \mathcal{D}$ fixed distribution $S \in \mathbb{R}^{d \times \tau}$

Costs $\tau \times O(\text{eval}(f_i))$ to evaluate $H_i(\theta)S$

Sketching and Projecting the Hessian: Action Matching (AM) approximation

find X such that

$$XS = H_i S$$

Sketching and Projecting the Hessian: Action Matching (AM) approximation

find X such that

$$XS = H_i S, \quad X = X^\top$$

Sketching and Projecting the Hessian: Action Matching (AM) approximation

$$\hat{H}_i = \arg\min_{X \in \mathbb{R}^{d\times d}} ||X||^2_{F(H)}$$

$$\text{subject to} \quad XS = H_i S, \quad X = X^\top$$

where $||X||^2_{F(H)} \overset{\text{def}}{=} \mathbf{Tr}\left(XHX^\top H\right)$ and $H = \nabla^2 f(\tilde{\theta})$

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$$\hat{H}_i = HS(S^T HS)^{-1} S^\top H_i \left(I - S(S^T HS)^{-1} S^\top H\right) + H_i S(S^T HS)^{-1} S^\top H.$$

Total inner iteration costs: $O\left(\tau \times \text{eval}(f_i) + \tau^2 d + \tau^3\right)$

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rank 2τ

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$$\frac{1}{n} \sum_{j=1}^{n} \hat{H}_j = HS(S^T HS)^{-1} S^\top H.$$

Total outer costs: $O(n\tau \times \text{eval}(f_i))$

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What about S ?

Total outer costs: $O(n\tau \times \text{eval}(f_i))$

Choosing the sketch matrix

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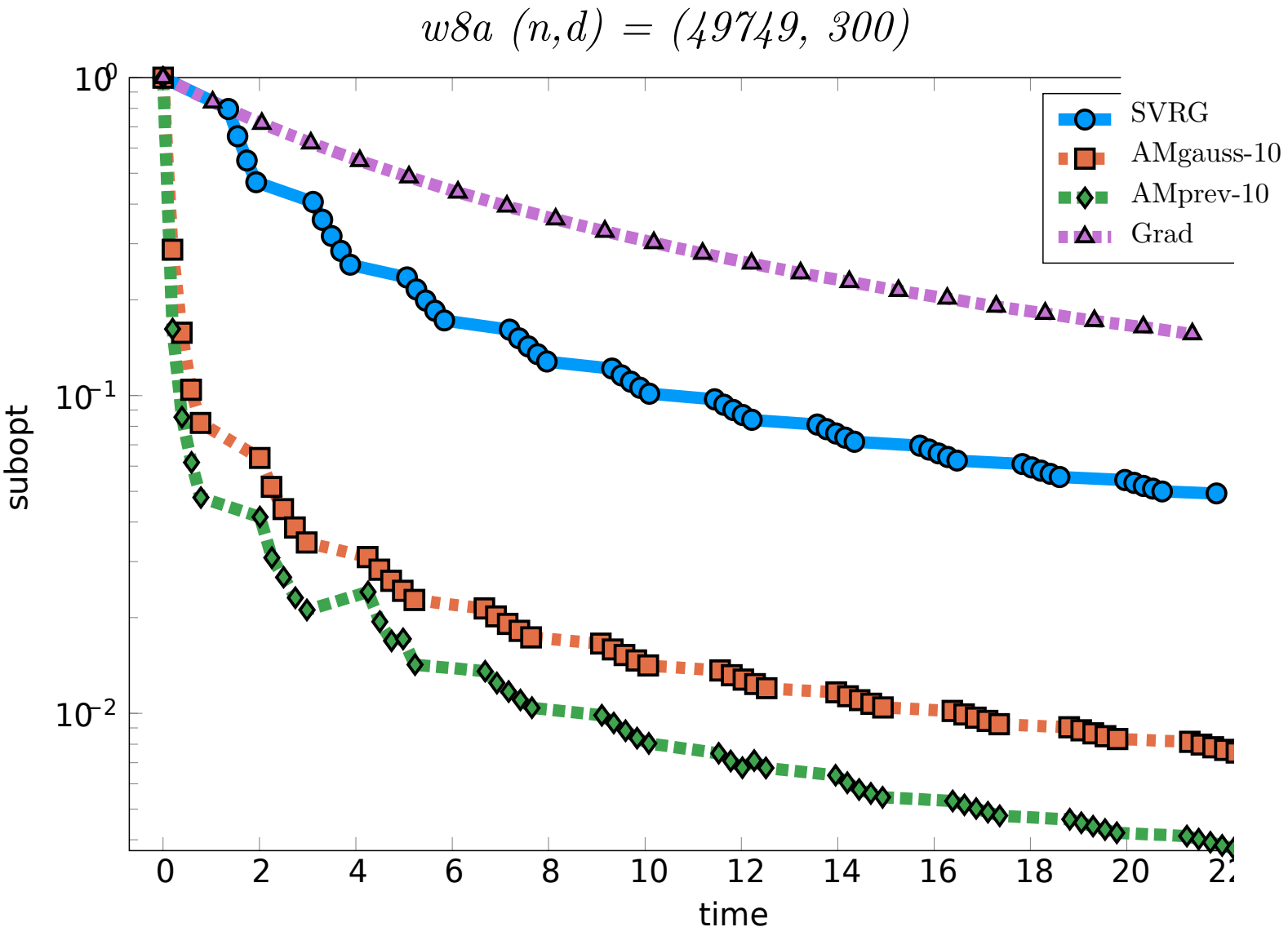
AMgauss: $S \sim \mathcal{N}(0, I)$ has Gaussian entries samplied i.i.d at each iteration

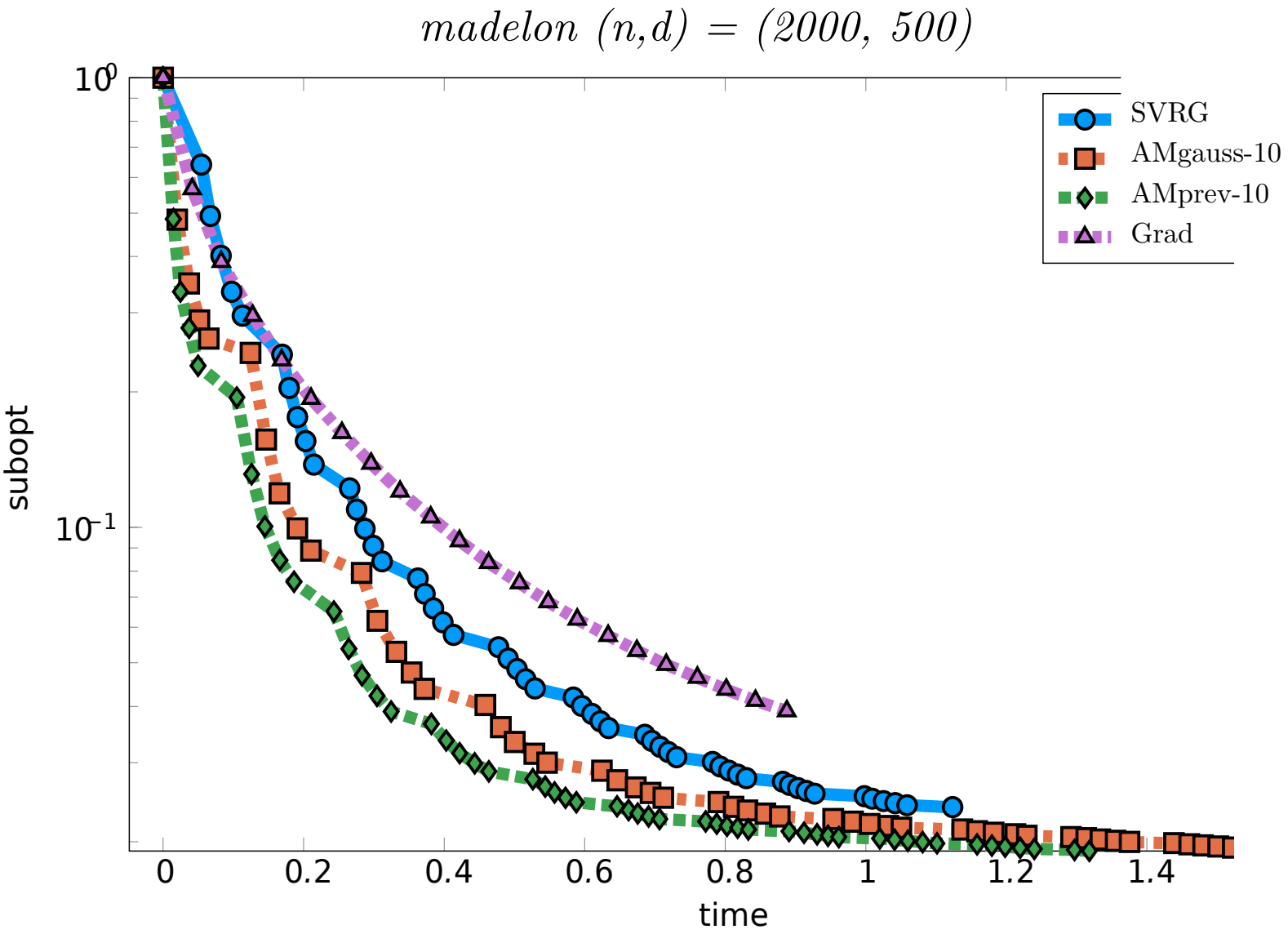
AMprev: Averages of **previous** search directions

$$S = [\bar{g}_0, \ldots, \bar{g}_{\tau-1}] \quad \text{where} \quad \bar{g}_i = \frac{\tau}{m} \sum_{j=\frac{m}{\tau} i}^{\frac{m}{\tau}(i+1)-1} g_j,$$

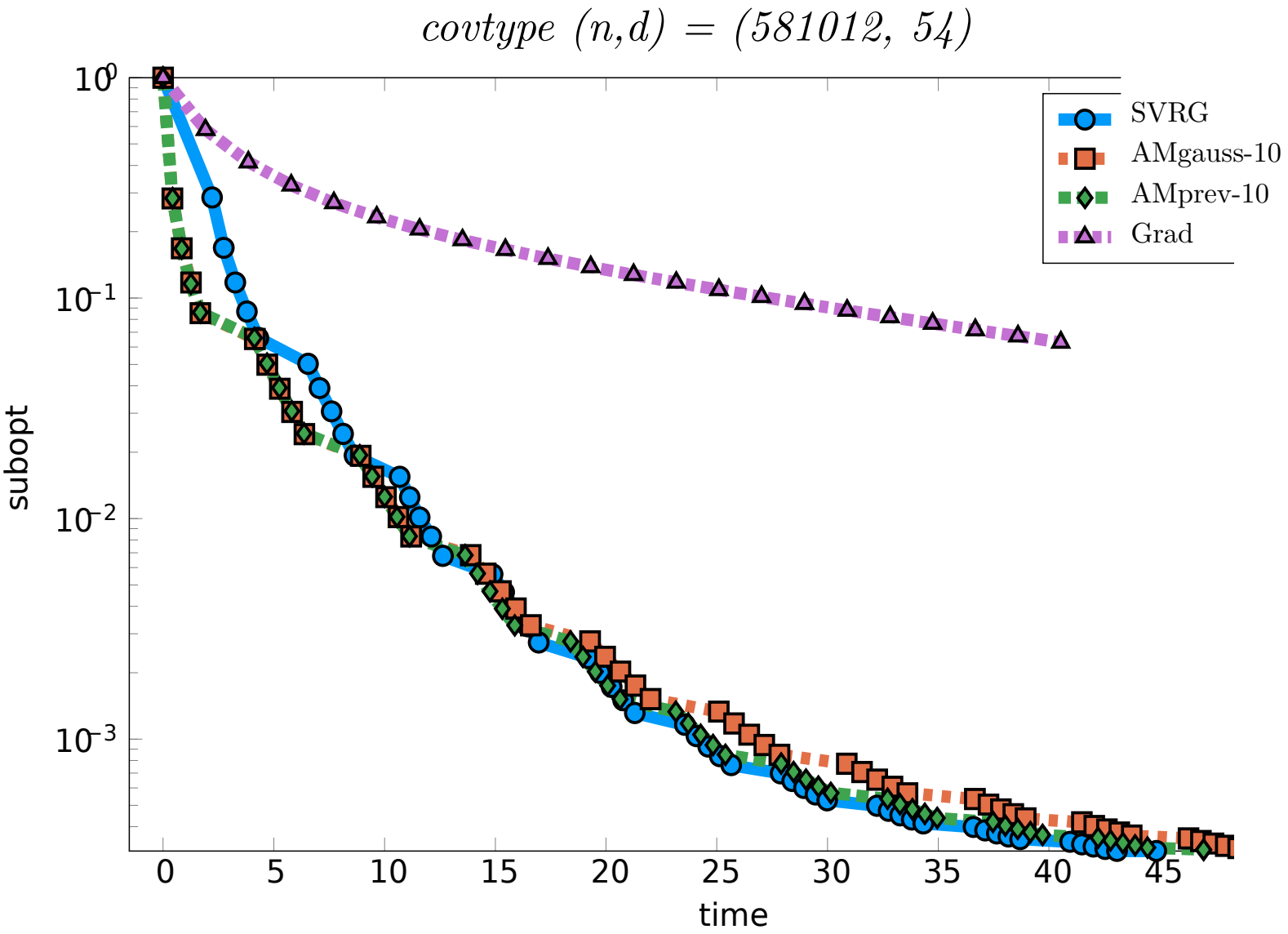
AM: Experiment works well



AM: Experiment works ok



AM: Experiment works badly



Take home:

Can use Hessian to diminish variance

Speed-ups with less gain and risk compared to Newton type methods.

New compressed Hessian estimates using sketching and projecting

gowerrobert/StochOpt.jl

Bruce Christianson. **Automatic Hessians by reverse accumulation**. In: IMA Journal of Numerical Analysis 12.2 (1992), pp. 135–150.

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D.. Goldfarb, (1970). **A Family of Variable-Metric Methods Derived by Variational Means**. Mathematics of Computation, 24(109), 23.