HiGrad: Statistical Inference for Online Learning and Stochastic Approximation

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Collaborator

- Yuancheng Zhu (Renaissance Technologies)

Learning by optimization

Sample $Z_1, \ldots, Z_N$, and $f(\theta, z)$ is cost function

Learning model by minimizing

$$\operatorname*{argmin}_{\theta} \frac{1}{N} \sum_{n=1}^{N} f(\theta, Z_n)$$

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- Maximum likelihood estimation (MLE). More generally, M-estimation
- Often no closed-form solution
- Need optimization

Gradient descent

- Start at some θ_0
- Iterate

$$\theta_j = \theta_{j-1} - \gamma_j \frac{\sum_{n=1}^{N} \nabla f(\theta_{j-1}, Z_n)}{N},$$

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However

- Offline algorithm
- Computational cost is high

Stochastic gradient descent (SGD)

Aka incremental gradient descent

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SGD resolved these challenges

- Online in nature
- One pass over data
- Optimal properties (Nemirovski & Yudin, 1983; Bertsekas, 1999; Agarwal et al, 2012; Rakhlin et al, 2012; Hardt et al, 2015)

SGD in one line

Using SGD for prediction

Averaged SGD

An estimator of $\theta^* := \operatorname{argmin} \mathbb{E} f(\theta, Z)$ is given by averaging

$$\overline{\theta} = \frac{1}{N} \sum_{j=1}^{N} \theta_j$$

Recall that $\theta_j = \theta_{j-1} - \gamma_j \nabla f(\theta_{j-1}, Z_j)$ for $j = 1, \ldots, N$.

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Given a new instance $z = (x, y)$ with y unknown

Interested in $\mu_x(\overline{\theta})$

- Linear regression: $\mu_x(\overline{\theta}) = x' \overline{\theta}$
- Logistic regression: $\mu_x(\overline{\theta}) = \frac{\mathrm{e}^{x' \overline{\theta}}}{1+\mathrm{e}^{x' \overline{\theta}}}$
- Generalized linear models: $\mu_x(\overline{\theta}) = \mathbb{E}_{\overline{\theta}}(Y|X = x)$

How much can we trust SGD predictions?

We would observe a different $\mu_x(\overline{\theta})$ if

- Re-sample $Z'_1, \ldots, Z'_N$
- Sample with replacement N times from a finite population

A real data example

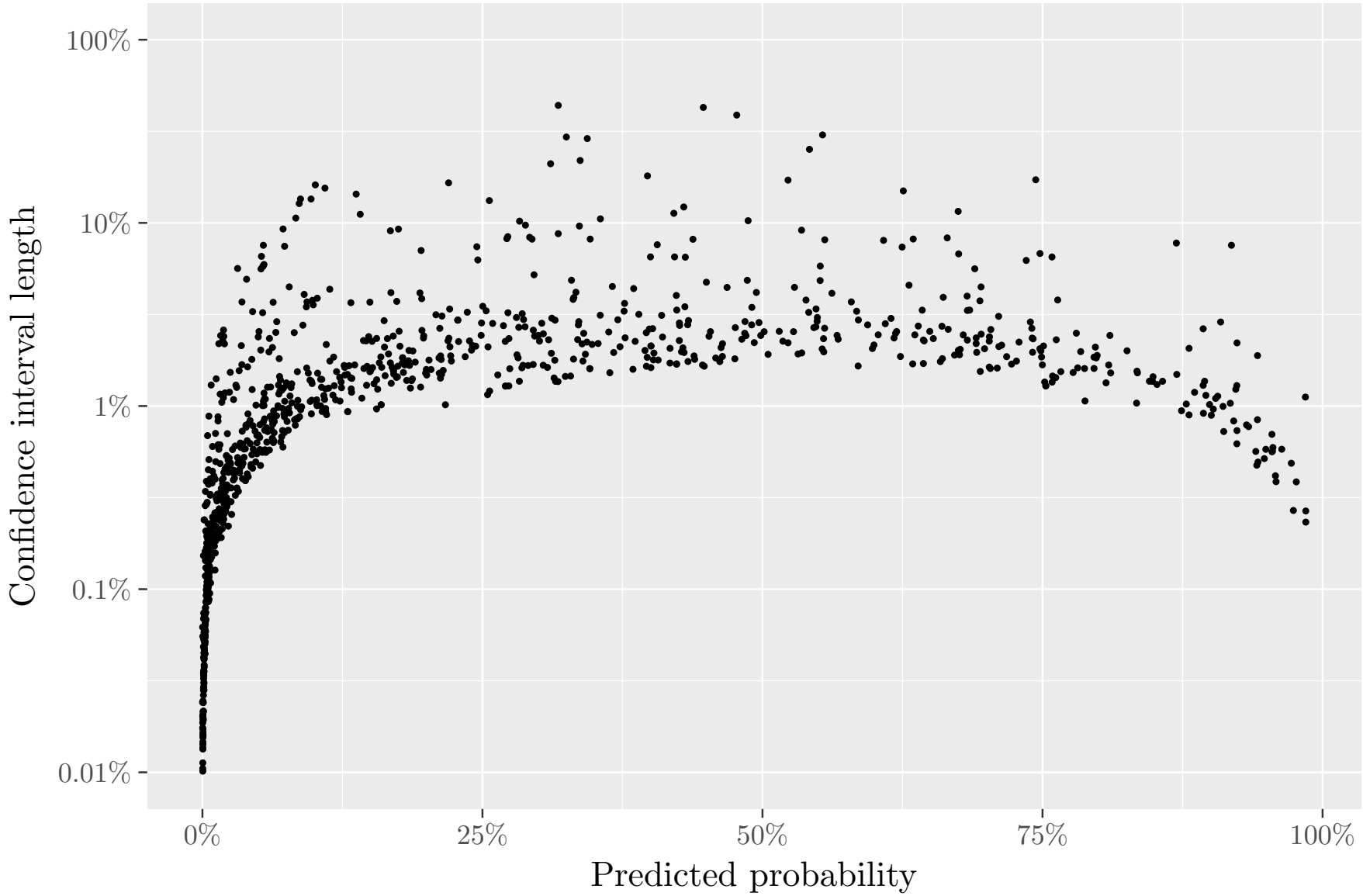
Adult dataset on UCI repository[1]

- 123 features
- $Y = 1$ if an individual's annual income exceeds \$50,000
- 32,561 instances

Randomly pick 1,000 as a test set. Run SGD 500 times independently, each with 20 epochs and step sizes $\gamma_j = 0.5j^{-0.55}$. Construct empirical confidence intervals with $\alpha = 10\%$

[1] `https://archive.ics.uci.edu/ml/datasets/Adult`

High variability of SGD predictions



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Can we construct a confidence interval for $\mu_x^* := \mu_x(\theta^*)$?

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Remarks

- Bootstrap is computationally infeasible
- Most existing works concern bounding generalization errors or minimizing regrets (Shalev-Shwartz et al, 2011; Rakhlin et al, 2012)
- Chen et al (2016) proposed a batch-mean estimator of SGD covariance, and Fang et al (2017) proposed a perturbation-based resampling procedure

This talk: HiGrad

A new method: Hierarchical Incremental GRAdient Descent

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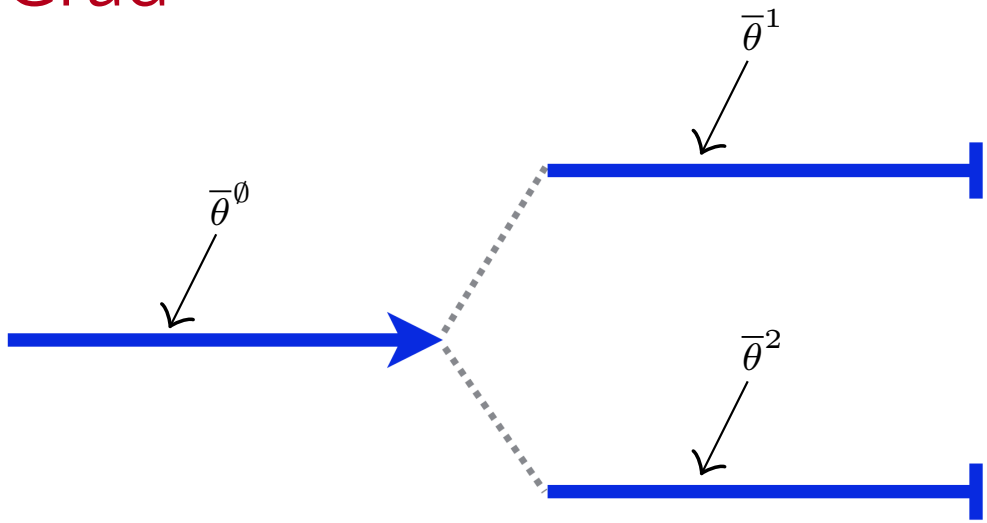
Preview of HiGrad



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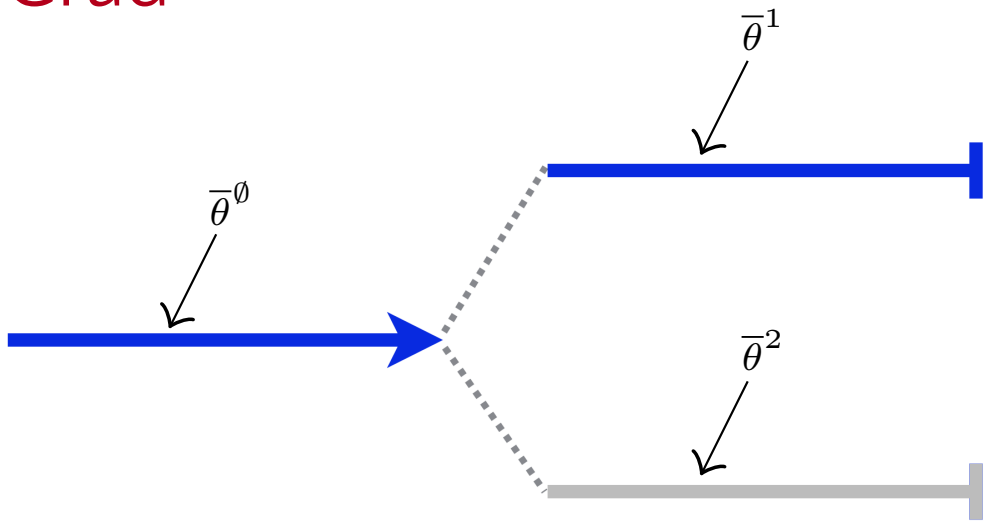

- $\overline{\theta}_1 = \frac{1}{3}\overline{\theta}^{\emptyset} + \frac{2}{3}\overline{\theta}^{1}, \quad \overline{\theta}_2 = \frac{1}{3}\overline{\theta}^{\emptyset} + \frac{2}{3}\overline{\theta}^{2}$

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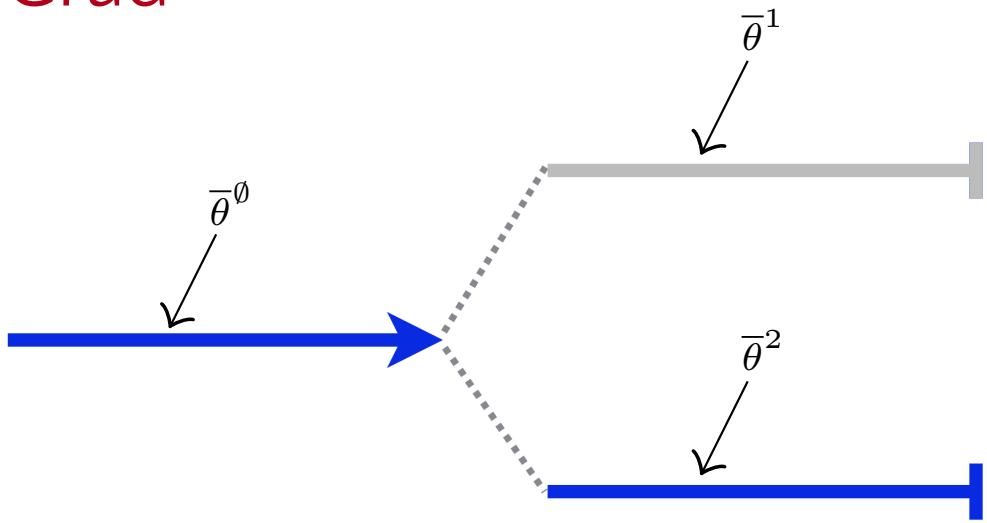

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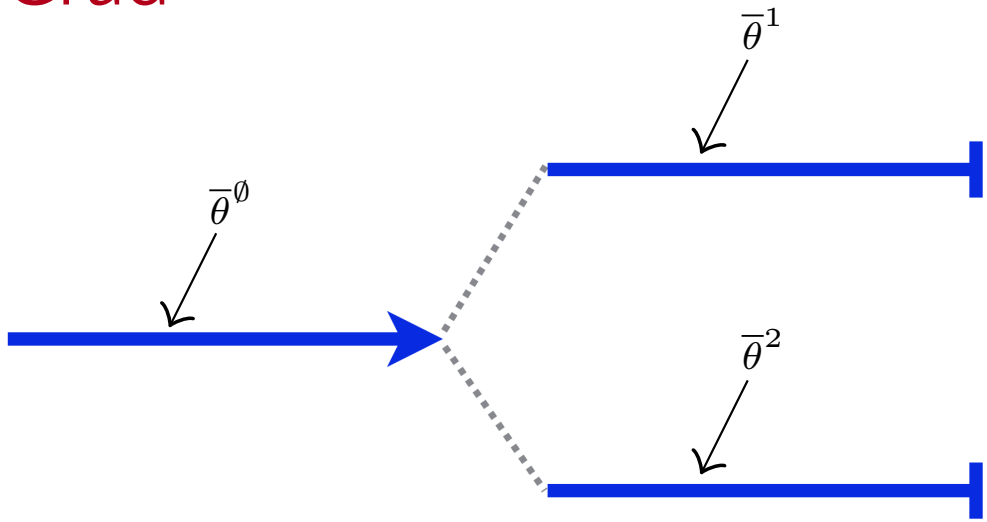

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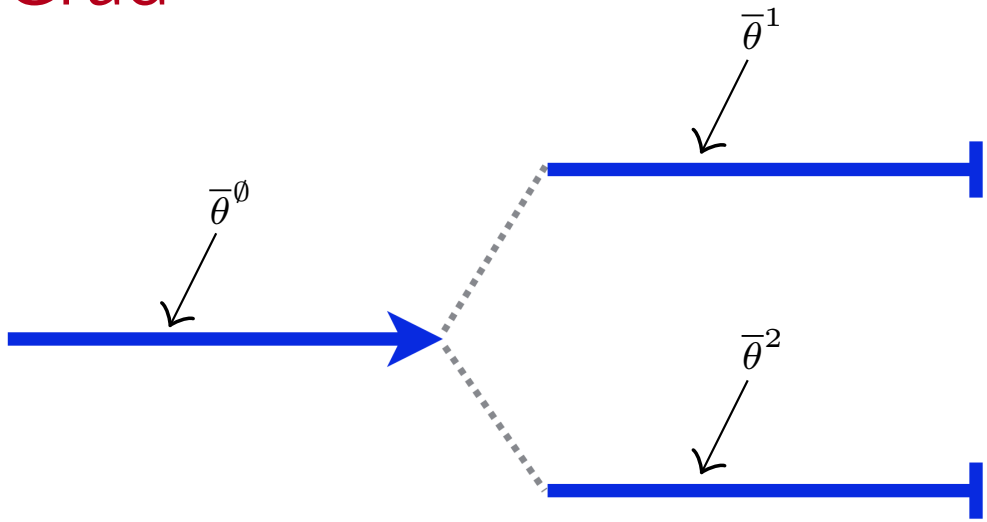

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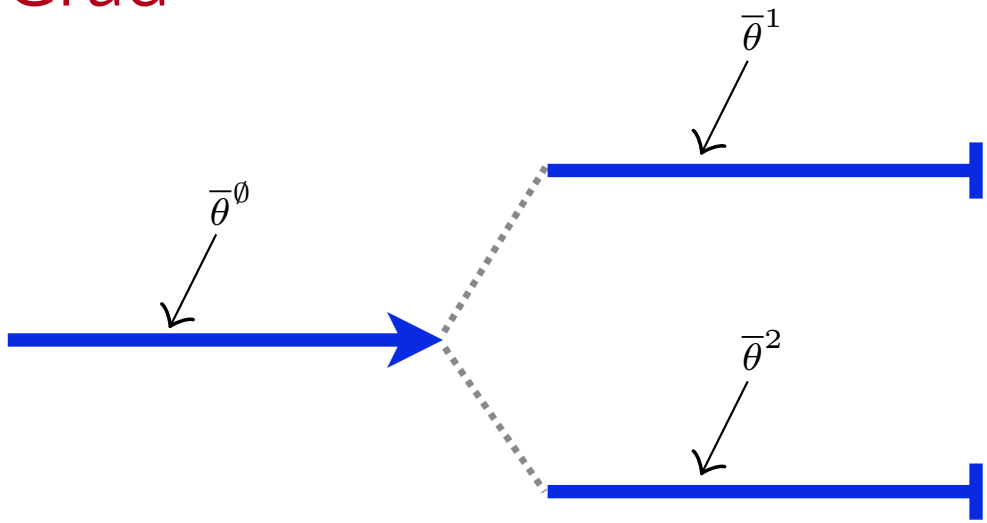

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- HiGrad estimator is $\overline{\mu}_x = \frac{\mu_x^1 + \mu_x^2}{2} = 0.13$
- The 90% HiGrad confidence interval for μ_x^* is

$$\left[\overline{\mu}_x - t_{1,0.95}\sqrt{0.375}|\mu_x^1 - \mu_x^2|,\ \overline{\mu}_x + t_{1,0.95}\sqrt{0.375}|\mu_x^1 - \mu_x^2|\right]$$
$$= [-0.025, 0.285]$$

Outline

Problem statement

Minimizing convex f

$$\theta^* = \operatorname*{argmin}_{\theta} \; f(\theta) \equiv \mathbb{E} f(\theta, Z)$$

Observe i.i.d. $Z_1, \ldots, Z_N$ and can evaluate unbiased noisy gradient $g(\theta; Z)$

$$\mathbb{E}\, g(\theta, Z) = \nabla f(\theta) \text{ for all } \theta$$

To be fulfilled

- Online in nature with same computational cost as vanilla SGD
- A confidence interval for μ_x^* in addition to an estimator
- Estimator (almost) as accurate as vanilla SGD

The idea of contrasting and sharing

- Need more than one value μ_x to quantify variability: **contrasting**

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- Need more than one value μ_x to quantify variability: **contrasting**
- Need to share gradient information to elongate threads: **sharing**

The HiGrad tree

- $K+1$ levels
- each k-level segment is of length n_k and is split into B_{k+1} segments

$$n_0 + B_1 n_1 + B_1 B_2 n_2 + B_1 B_2 B_3 n_3 + \cdots + B_1 B_2 \cdots B_K n_K = N$$

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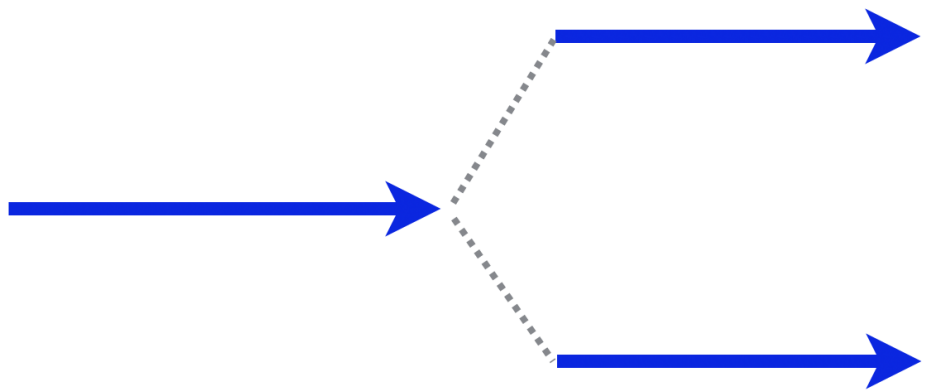

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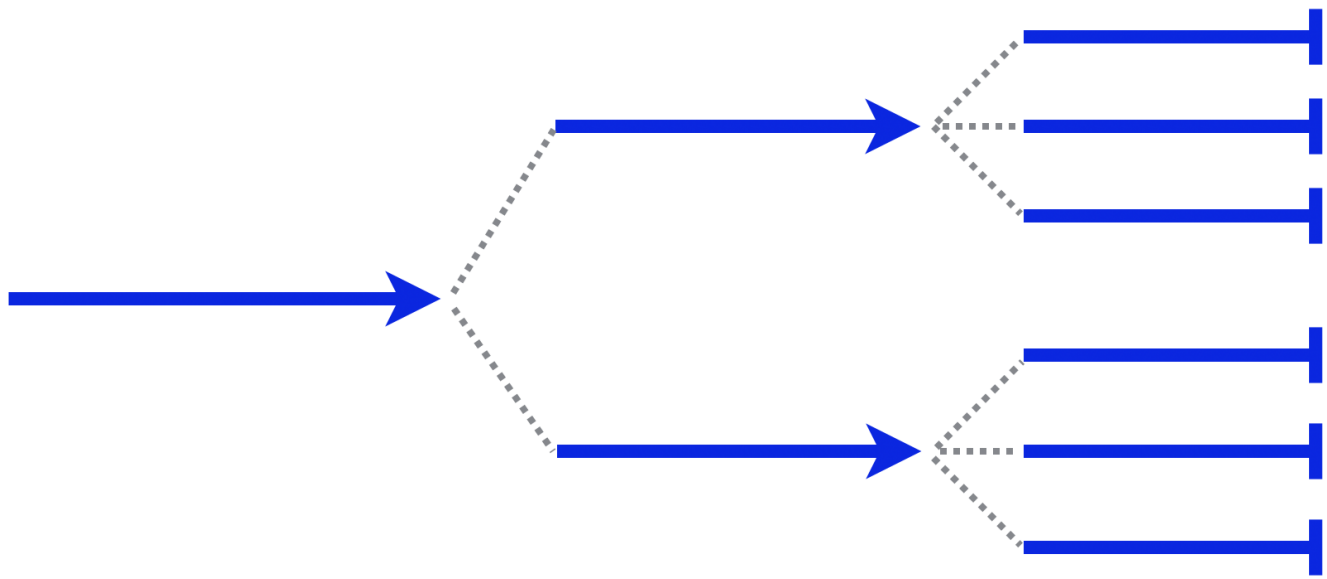

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Iterate along HiGrad tree

Recall: noisy gradient $g(\theta, Z)$ unbiased for $\nabla f(\theta)$; partition $\{Z^{\boldsymbol{s}}\}$ of $\{Z_1, \ldots, Z_N\}$; and $L_k := n_0 + \cdots + n_k$

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- Iterate along each level 1 segment $\boldsymbol{s} = (b_1)$ for $1 \leq b_1 \leq B_1$

$$\theta_j^{\boldsymbol{s}} = \theta_{j-1}^{\boldsymbol{s}} - \gamma_{j+L_0} g(\theta_{j-1}^{\boldsymbol{s}}, Z_j^{\boldsymbol{s}})$$

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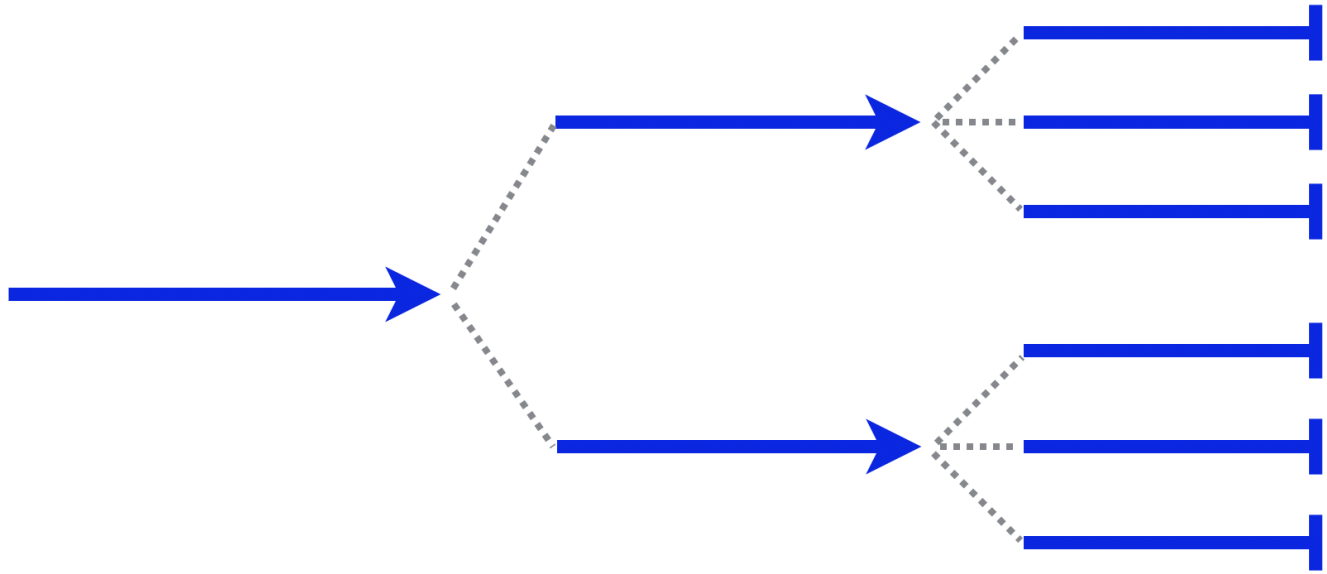
  for $j = 1, \ldots, n_1$, starting from θ_{n_0}
- Generally, for the segment $\boldsymbol{s} = (b_1 \cdots b_k)$, iterate

$$\theta_j^{\boldsymbol{s}} = \theta_{j-1}^{\boldsymbol{s}} - \gamma_{j+L_{k-1}}\, g(\theta_{j-1}^{\boldsymbol{s}}, Z_j^{\boldsymbol{s}})$$

  for $j = 1, \ldots, n_k$, starting from $\theta_{n_{k-1}}^{(b_1 \cdots b_{k-1})}$

A second look at the HiGrad tree



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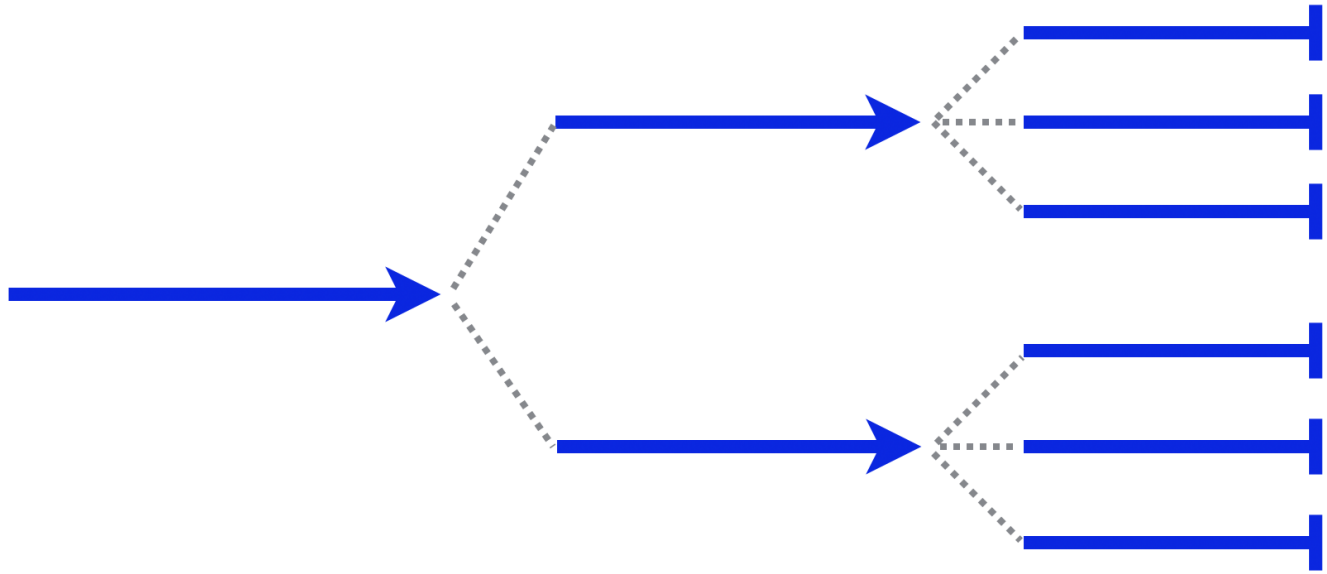

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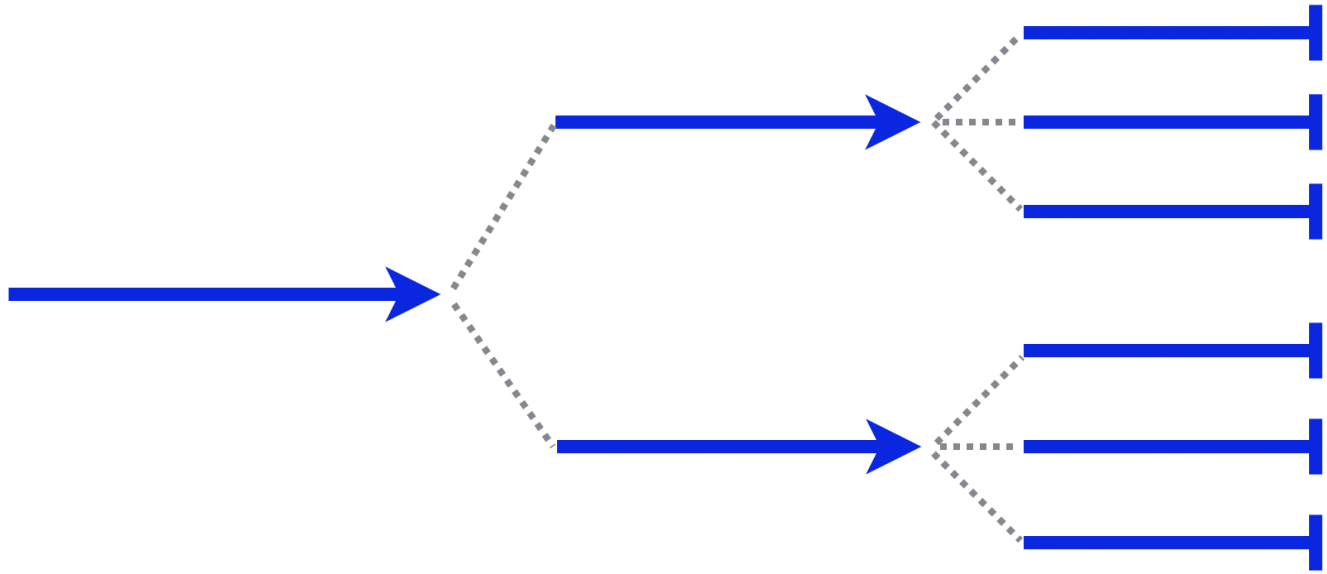

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Bonus

Easier to parallelize than vanilla SGD!

Outline

Estimate μ_x^* through each thread

Average over each segment $\boldsymbol{s} = (b_1, \ldots, b_k)$

$$\overline{\theta}^{\boldsymbol{s}} = \frac{1}{n_k} \sum_{j=1}^{n_k} \theta_j^{\boldsymbol{s}}$$

Given weights $w_0, w_1, \ldots, w_K$ that sum up to 1, weighted average along thread $\boldsymbol{t} = (b_1, \ldots, b_K)$ is

$$\overline{\theta}_{\boldsymbol{t}} = \sum_{k=0}^{K} w_k \overline{\theta}^{(b_1, \ldots, b_k)}$$

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Estimator yielded by thread t

$$\mu_x^{\boldsymbol{t}} := \mu_x(\overline{\theta}_{\boldsymbol{t}})$$

How to construct a confidence interval based on $T := B_1 B_2 \cdots B_K$ many such μ_x^t estimates?

Assume normality

Denote by $\boldsymbol{\mu}_x$ the T-dimensional vector consisting of all $\mu_x^{\boldsymbol{t}}$

Normality of $\boldsymbol{\mu}_x$ (to be shown later)

$\sqrt{N}(\boldsymbol{\mu}_x - \mu_x^* \mathbf{1})$ converges weakly to normal distribution $\mathcal{N}(\mathbf{0}, \Sigma)$ as $N \to \infty$

Convert to simple linear regression

From $\boldsymbol{\mu}_x \overset{a}{\sim} \mathcal{N}(\mu_x^* \mathbf{1}, \Sigma/N)$ we get

$$\Sigma^{-\frac{1}{2}} \boldsymbol{\mu}_x \approx (\Sigma^{-\frac{1}{2}} \mathbf{1}) \mu_x^* + \tilde{\boldsymbol{z}}, \quad \tilde{\boldsymbol{z}} \sim \mathcal{N}(0, \boldsymbol{I}/N)$$

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Simple linear regression! Least-squares estimator of μ_x^* given as

$$\begin{aligned}
&(\mathbf{1}' \Sigma^{-\frac{1}{2}} \Sigma^{-\frac{1}{2}} \mathbf{1})^{-1} \mathbf{1}' \Sigma^{-\frac{1}{2}} \Sigma^{-\frac{1}{2}} \boldsymbol{\mu}_x \\
&= (\mathbf{1}' \Sigma^{-1} \mathbf{1})^{-1} \mathbf{1}' \Sigma^{-1} \boldsymbol{\mu}_x \\
&= \frac{1}{T} \sum_{\boldsymbol{t} \in \mathcal{T}} \mu_x^{\boldsymbol{t}} \equiv \overline{\mu}_x
\end{aligned}$$

HiGrad estimator

Just the sample mean $\overline{\mu}_x$

A t-based confidence interval

A *pivot* for μ_x^*

$$\frac{\overline{\mu}_x - \mu_x^*}{\mathrm{SE}_x} \overset{a}{\sim} t_{T-1},$$

where the standard error is given as

$$\mathrm{SE}_x = \sqrt{\frac{(\boldsymbol{\mu}_x' - \overline{\mu}_x \mathbf{1}')\Sigma^{-1}(\boldsymbol{\mu}_x - \overline{\mu}_x \mathbf{1})}{T-1}} \cdot \frac{\sqrt{\mathbf{1}'\Sigma\mathbf{1}}}{T}$$

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HiGrad confidence interval of coverage $1-\alpha$

$$\left[\overline{\mu}_x - t_{T-1,1-\frac{\alpha}{2}}\,\mathrm{SE}_x, \quad \overline{\mu}_x + t_{T-1,1-\frac{\alpha}{2}}\,\mathrm{SE}_x\right]$$

Do we know the covariance Σ?

An extension of Ruppert–Polyak normality

Given a thread $\boldsymbol{t} = (b_1, \ldots, b_K)$, denote by segments $\boldsymbol{s}_k = (b_1, b_2, \ldots, b_k)$

Fact (informal)

$\sqrt{n_0}(\overline{\theta}^{\boldsymbol{s}_0} - \theta^*), \sqrt{n_1}(\overline{\theta}^{\boldsymbol{s}_1} - \theta^*), \ldots, \sqrt{n_K}(\overline{\theta}^{\boldsymbol{s}_K} - \theta^*)$ converge to i.i.d. centered normal distributions

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- Hessian $H = \nabla^2 f(\theta^*)$ and $V = \mathbb{E}\left[g(\theta^*, Z)g(\theta^*, Z)'\right]$. Ruppert (1988), Polyak (1990), and Polyak and Juditsky (1992) prove

$$\sqrt{N}(\overline{\theta}_N - \theta^*) \Rightarrow \mathcal{N}(0, H^{-1}VH^{-1})$$

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- *To know covariance of $\{\mu_x(\overline{\theta}_{\boldsymbol{t}})\}$, really need to know $H^{-1}VH^{-1}$?*

Covariance determined by number of shared segments

Lemma

For any two threads $\boldsymbol{t}$ and $\boldsymbol{t}'$ that agree at the first k segments and differ henceforth, we have

$$\operatorname{Cov}\left(\mu_x^{\boldsymbol{t}}, \mu_x^{\boldsymbol{t}'}\right) = (1 + o(1))\sigma^2 \sum_{i=0}^{k} \frac{w_i^2}{n_i}$$

Specify Σ up to a multiplicative factor

$$\Sigma_{\boldsymbol{t},\boldsymbol{t}'} = (1 + o(1))C \sum_{i=0}^{k} \frac{\omega_i^2 N}{n_i}$$

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- Do we need to know C as well?

Specify Σ up to a multiplicative factor

$$\Sigma_{\boldsymbol{t},\boldsymbol{t}'} = (1 + o(1))C \sum_{i=0}^{k} \frac{\omega_i^2 N}{n_i}$$

- Do we need to know C as well?
- No! Standard error of $\overline{\mu}_x$ invariant under multiplying Σ by a scalar

$$\mathrm{SE}_x = \sqrt{\frac{(\boldsymbol{\mu}_x' - \overline{\mu}_x \mathbf{1}')\Sigma^{-1}(\boldsymbol{\mu}_x - \overline{\mu}_x \mathbf{1})}{T-1}} \cdot \frac{\sqrt{\mathbf{1}'\Sigma\mathbf{1}}}{T}$$

Formal statement of theoretical results

Assumptions

1. **Local strong convexity.** $f(\theta) \equiv \mathbb{E} f(\theta, Z)$ *convex*, differentiable, with Lipschitz gradients. Hessian $\nabla^2 f(\theta)$ locally Lipschitz and *positive-definite* at θ^*

2. **Noise regularity.** $V(\theta) = \mathbb{E}\left[g(\theta, Z) g(\theta, Z)'\right]$ Lipschitz and does not grow too fast. Noisy gradient $g(\theta, Z)$ has $2 + o(1)$ moment locally at θ^*

Examples satisfying assumptions

- **Linear regression**: $f(\theta, z) = \frac{1}{2}(y - x^\top \theta)^2$.
- **Logistic regression**: $f(\theta, z) = -yx^\top \theta + \log\left(1 + \mathrm{e}^{x^\top \theta}\right)$.
- **Penalized regression**: Add a ridge penalty $\lambda\|\theta\|^2$.
- **Huber regression**: $f(\theta, z) = \rho_\lambda(y - x^\top \theta)$, where $\rho_\lambda(a) = a^2/2$ for $|a| \leq \lambda$ and $\rho_\lambda(a) = \lambda|a| - \lambda^2/2$ otherwise.

Sufficient conditions

X in *generic* position, and $\mathbb{E}\|X\|^{4+o(1)} < \infty$ and $\mathbb{E}|Y|^{2+o(1)}\|X\|^{2+o(1)} < \infty$

Main theoretical results

Theorem (S. and Zhu)

Assume K and $B_1, \ldots, B_K$ are fixed, $n_k \propto N$ as $N \to \infty$, and μ_x has a nonzero derivative at θ^*. Taking $\gamma_j \asymp j^{-\alpha}$ for $\alpha \in (0.5, 1)$ gives

$$\frac{\overline{\mu}_x - \mu_x^*}{\mathrm{SE}_x} \Longrightarrow t_{T-1}$$

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Confidence intervals

$$\lim_{N \to \infty} \mathbb{P}\left(\mu_x^* \in \left[\overline{\mu}_x - t_{T-1,1-\frac{\alpha}{2}}\,\mathrm{SE}_x, \quad \overline{\mu}_x + t_{T-1,1-\frac{\alpha}{2}}\,\mathrm{SE}_x\right]\right) = 1 - \alpha$$

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Fulfilled

- Online in nature with same computational cost as vanilla SGD ✓
- A confidence interval for μ_x^* in addition to an estimator ✓

How accurate is the HiGrad estimator?

Optimal variance with optimal weights

By Cauchy–Schwarz

$$N\,\mathbb{V}\mathsf{ar}(\overline{\mu}_x) = (1+o(1))\sigma^2 \left[\sum_{k=0}^{K} n_k \prod_{i=1}^{k} B_i\right] \left[\sum_{k=0}^{K} \frac{w_k^2}{n_k \prod_{i=1}^{k} B_i}\right]$$
$$\geq (1+o(1))\sigma^2 \left[\sum_{k=0}^{K} \sqrt{w_k^2}\right]^2 = (1+o(1))\sigma^2,$$

with equality if

$$w_k^* = \frac{n_k \prod_{i=1}^{k} B_i}{N}$$

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- Segments at an early level are weighted less

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- HiGrad estimator has the *same* asymptotic variance as vanilla SGD

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- Segments at an early level are weighted less
- HiGrad estimator has the *same* asymptotic variance as vanilla SGD
- Achieves Cramér–Rao lower bound when model specified

Prediction intervals for vanilla SGD

Theorem (S. and Zhu)

Run vanilla SGD on a fresh dataset of the same size, producing μ_x^{SGD}. Then, with optimal weights,

$$\lim_{N\to\infty} \mathbb{P}\left(\mu_x^{\mathrm{SGD}} \in \left[\overline{\mu}_x - \sqrt{2}t_{T-1,1-\frac{\alpha}{2}}\,\mathrm{SE}_x, \quad \overline{\mu}_x + \sqrt{2}t_{T-1,1-\frac{\alpha}{2}}\,\mathrm{SE}_x\right]\right) = 1-\alpha.$$

- μ_x^{SGD} can be replaced by the HiGrad estimator with the same structure
- Interpretable even under model misspecification

Three properties

Under certain assumptions, for example, f being locally strongly convex

Fulfilled

- Online in nature with same computational cost as vanilla SGD 
- A confidence interval for μ_x^* in addition to an estimator
- Estimator (almost) as accurate as vanilla SGD

Outline

General simulation setup

X generated as i.i.d. $\mathcal{N}(0,1)$ and $Z = (X, Y) \in \mathbb{R}^d \times \mathbb{R}$. Set $N = 10^6$ and use $\gamma_j = 0.5j^{-0.55}$

- Linear regression $Y \sim \mathcal{N}(\mu_X(\theta^*), 1)$, where $\mu_x(\theta) = x'\theta$
- Logistic regression $Y \sim \text{Bernoulli}(\mu_X(\theta^*))$, where

$$\mu_x(\theta) = \frac{\mathrm{e}^{x'\theta}}{1 + \mathrm{e}^{x'\theta}}$$

Criteria

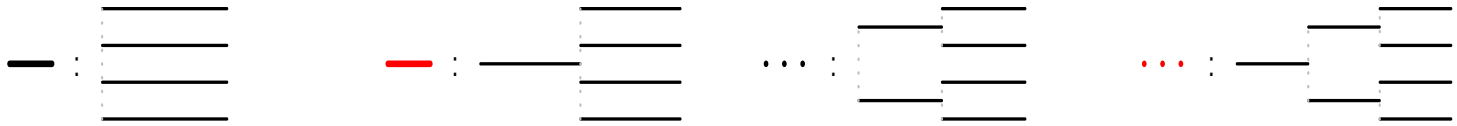
- Accuracy: $\|\overline{\theta} - \theta^*\|^2$, where $\overline{\theta}$ averaged over T threads
- Coverage probability and length of confidence interval

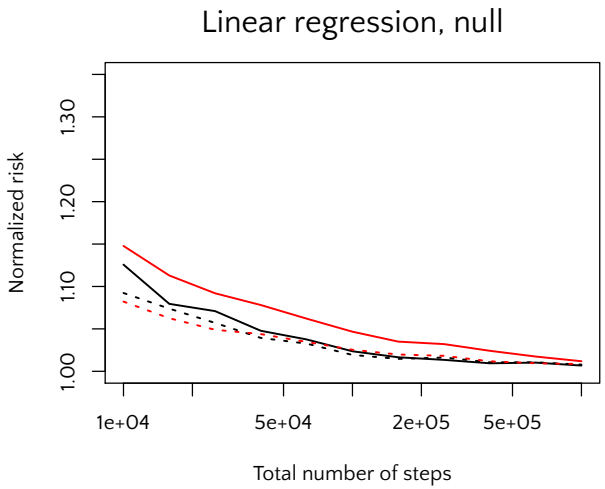
Accuracy

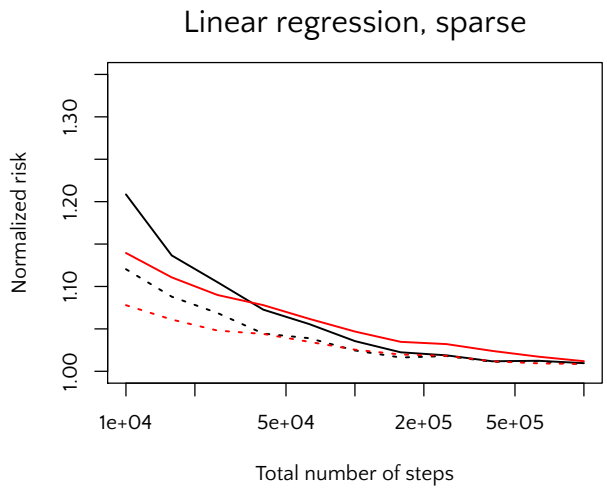
Dimension $d = 50$. MSE $\|\overline{\theta} - \theta^*\|^2$ normalized by that of vanilla SGD

- *null* case where $\theta_1 = \cdots = \theta_{50} = 0$
- *dense* case where $\theta_1 = \cdots = \theta_{50} = \frac{1}{\sqrt{50}}$
- *sparse* case where $\theta_1 = \cdots = \theta_5 = \frac{1}{\sqrt{5}}$, $\theta_6 = \cdots = \theta_{50} = 0$

Accuracy




Linear regression, null
Normalized risk
1.00
1.10
1.20
1.30
1e+04
5e+04
2e+05
5e+05
Total number of steps


Linear regression, sparse
Normalized risk
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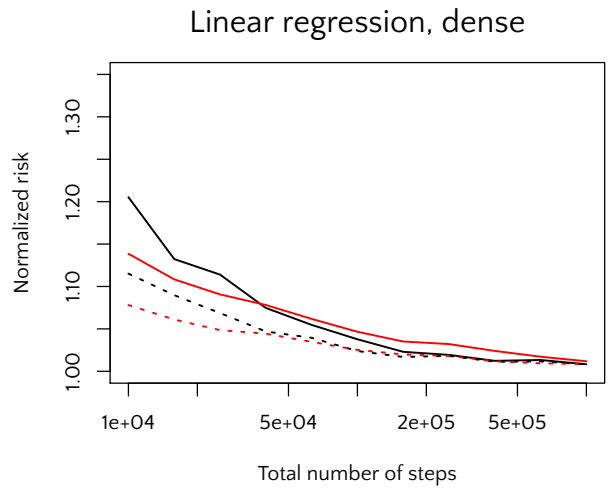
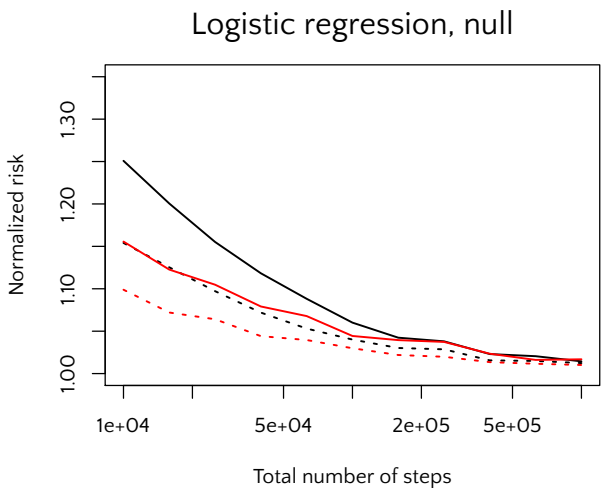
1.10
1.20
1.30
1e+04
5e+04
2e+05
5e+05
Total number of steps


Linear regression, dense
Normalized risk
1.00
1.10
1.20
1.30
1e+04
5e+04
2e+05
5e+05
Total number of steps


Logistic regression, null
Normalized risk
1.00
1.10
1.20
1.30
1e+04
5e+04
2e+05
5e+05
Total number of steps


Logistic regression, sparse
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1.00
1.10
1.20
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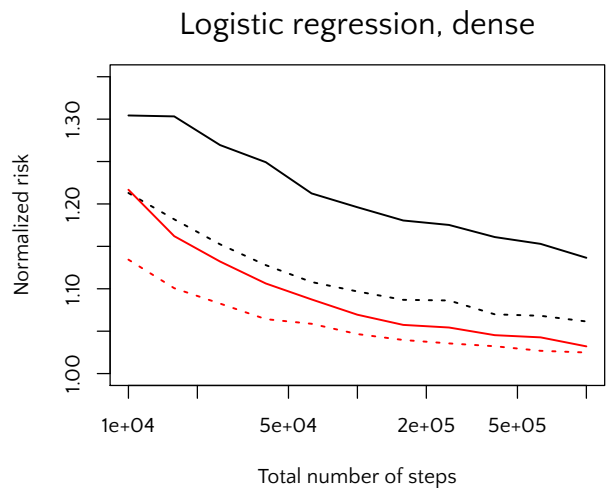
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1.00
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1.30
1e+04
5e+04
2e+05
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Total number of steps

Coverage and CI length

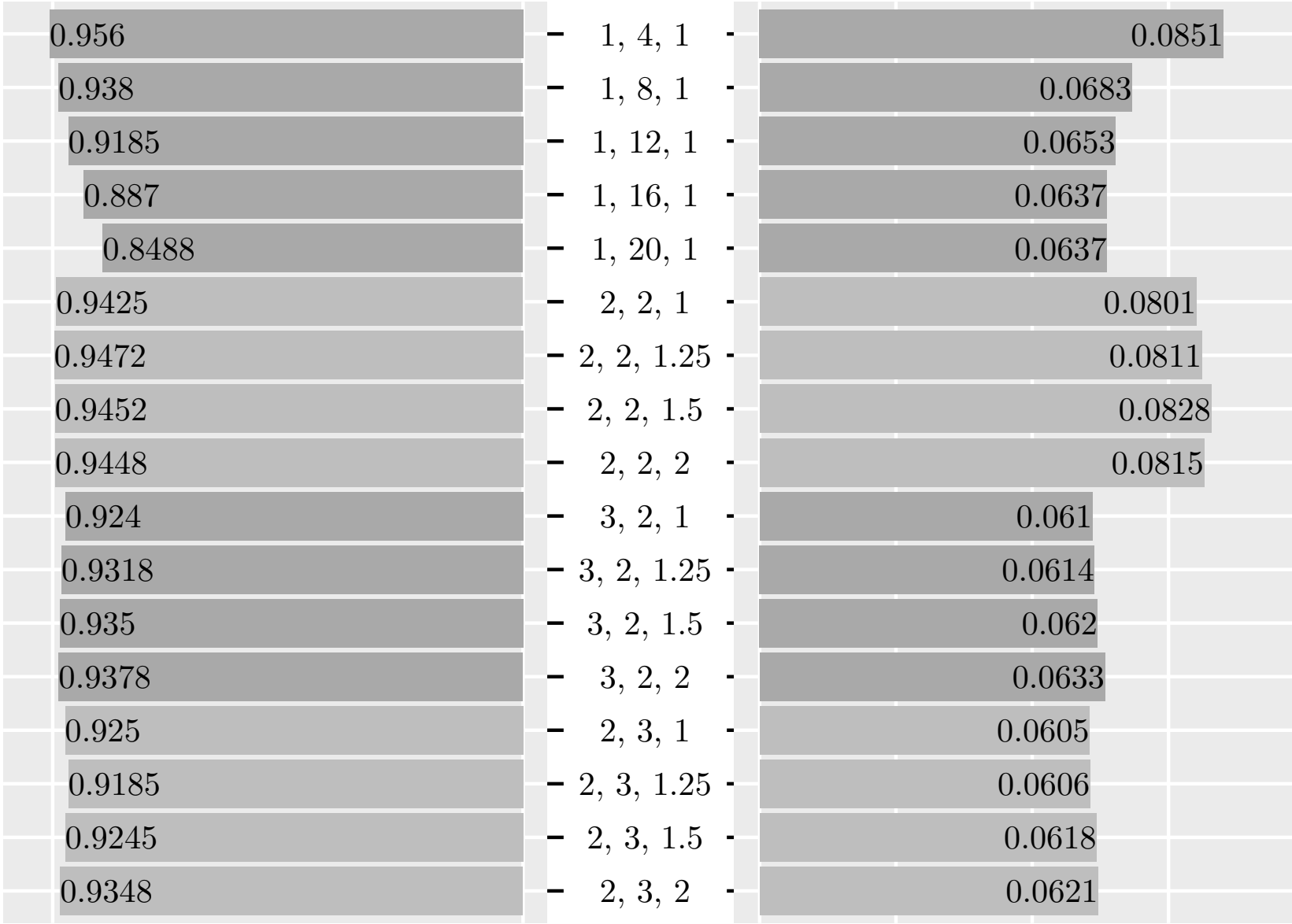
HiGrad configurations

- $K = 1$, then $n_1/n_0 = r = 1$;
- $K = 2$, then $n_1/n_0 = n_2/n_1 = r \in \{0.75, 1, 1.25, 1.5\}$

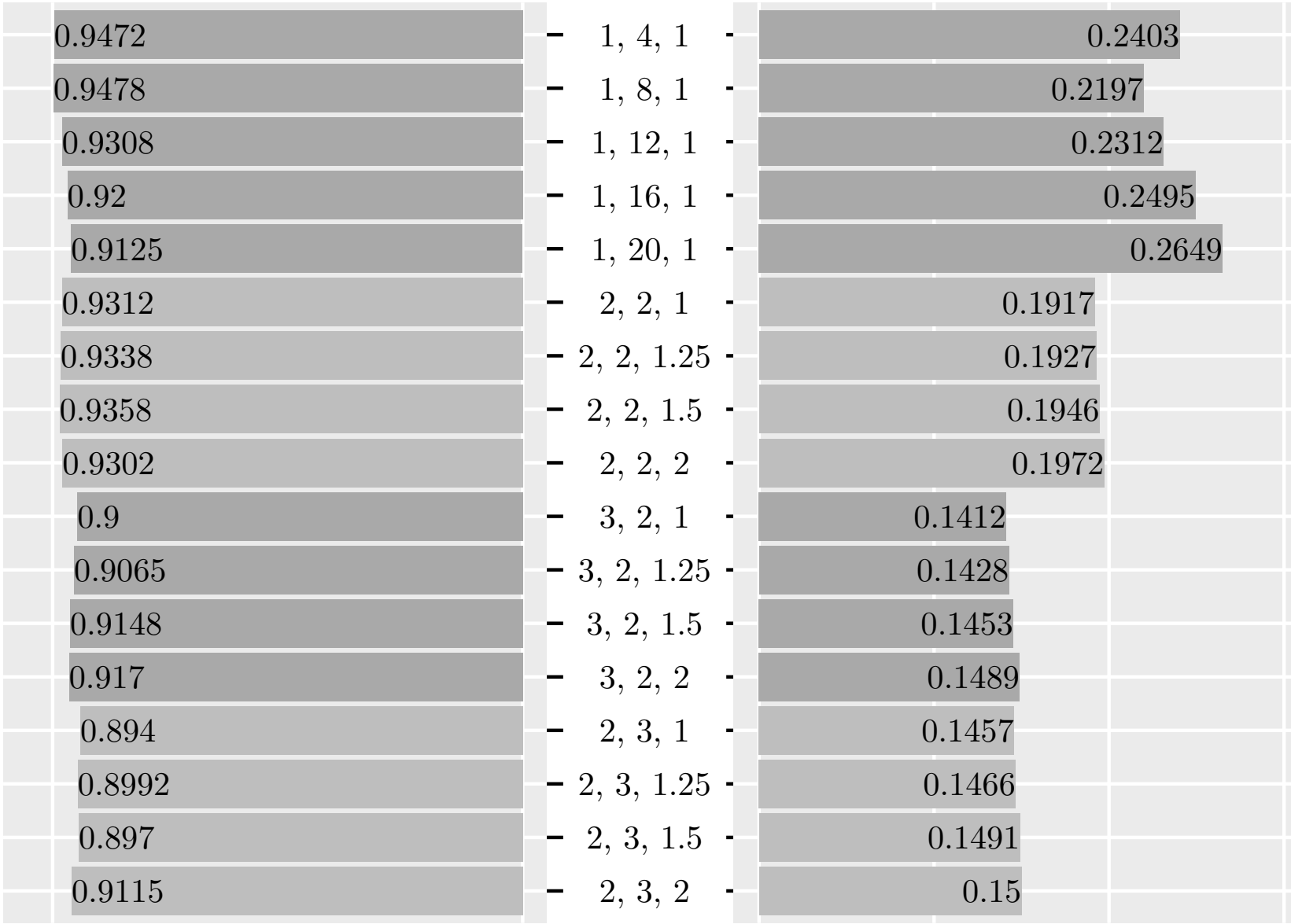
Set $\theta_i^* = (i-1)/d$ for $i = 1, \ldots, d$ and $\alpha = 5\%$. Use measure

$$\frac{1}{20} \sum_{i=1}^{20} \mathbf{1}(\mu_{x_i}(\theta^*) \in \mathsf{CI}_{x_i})$$

Linear regression: $d = 20$



Linear regression: $d = 100$



A real data example: setup

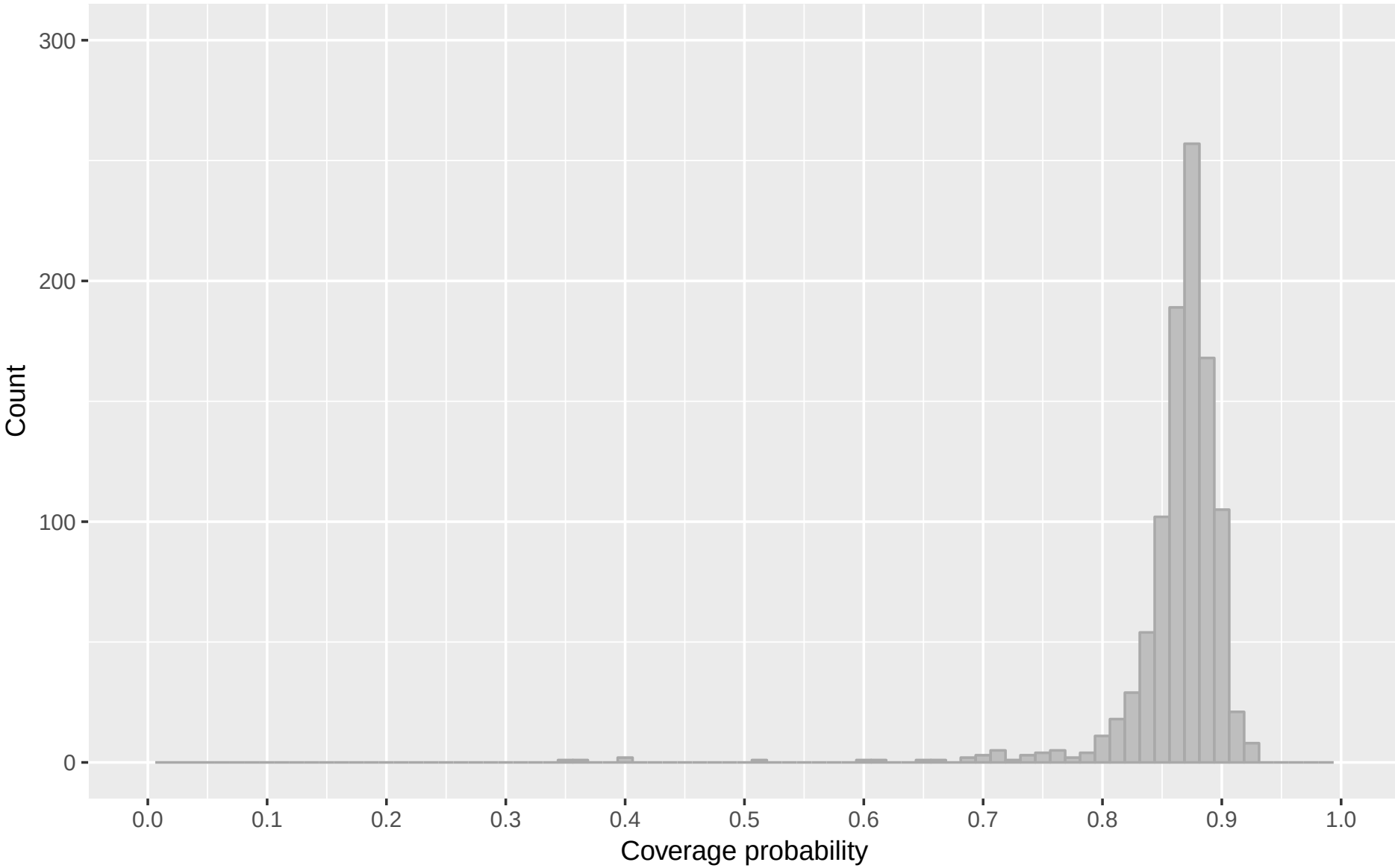
From the 1994 census data based on UCI repository. Y indicates if an individual's annual income exceeds \$50,000

- 123 features
- 32,561 instances
- Randomly pick 1,000 as a test set

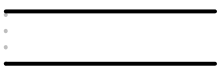
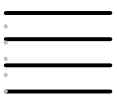
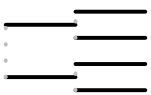
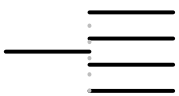
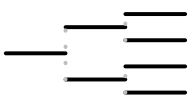
Use $N = 10^6, \alpha = 10\%$, and $\gamma_j = 0.5j^{-0.55}$. Run HiGrad for $L = 500$ times. Use measure

$$\text{coverage}_i = \frac{1}{L(L-1)} \sum_{\ell_1}^{L} \sum_{\ell_2 \neq \ell_1} \mathbf{1}\left(\hat{p}_{i\ell_1} \in \text{PI}_{i\ell_2}\right)$$

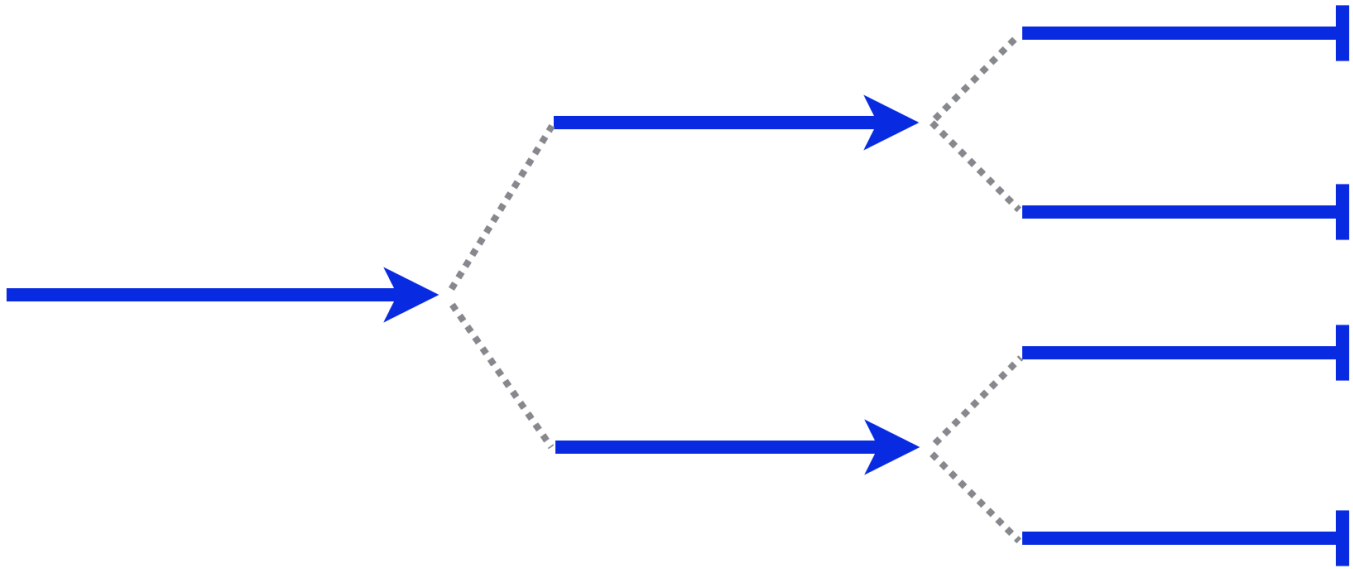
A real data example: histogram



Comparisons of HiGrad configurations

Configurations	Accuracy	Coverage	CI length
	★★★★★	☆☆☆☆☆	☆☆☆☆☆
	★★★★☆	★★★★★	★★☆☆☆
	★★★☆☆	★★★★½	★★★★☆
	★★★½☆	★★★★☆	★★★★☆
	★★★½☆	★★★★☆	★★★★☆
	★★★★☆	★★★★☆	★★★★☆

Default HiGrad parameters



`HiGrad` R package default values

$$K = 2, B_1 = 2, B_2 = 2, n_0 = n_1 = n_2 = \frac{N}{7}$$

Concluding Remarks

Possible extensions

Improving statistical properties

- Finite-sample guarantee
  - Better coverage probability

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  - Better coverage probability
- Extend Ruppert-Polyak to high dimensions
  - Number of unknown variables growing

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A new template for online learning

- Non-convex problems
  - Online PCA, stochastic EM, etc

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A new template for online learning

- Non-convex problems
  - Online PCA, stochastic EM, etc
- A criterion for early stopping
  - Detect overfitting through contrasting
  - Need to incorporate selective inference
- Any ideas? Happy to talk offline

Take-home messages

Idea

Contrasting and sharing through hierarchical splitting

Take-home messages

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Contrasting and sharing through hierarchical splitting

Properties (local strong convexity)

- Online in nature with same computational cost as vanilla SGD
- A confidence interval for μ_x^* in addition to an estimator
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Contrasting and sharing through hierarchical splitting

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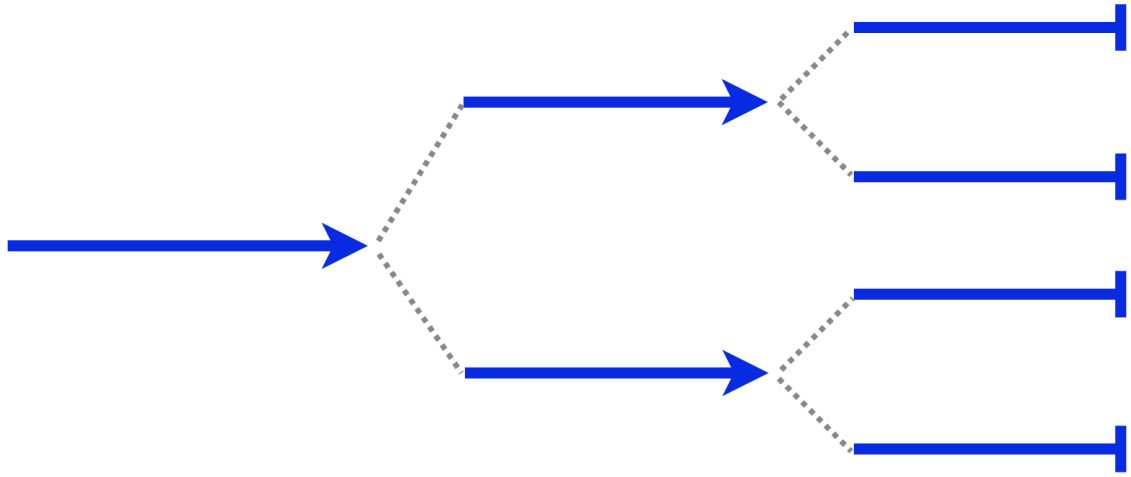
Bonus

Easier to parallelize than vanilla SGD!

Thanks!



- **Reference.** *Statistical Inference for Online Learning and Stochastic Approximation via Hierarchical Incremental Gradient Descent*, Weijie J. Su and Yuancheng Zhu, arXiv paper
- **Software.** R package `higrad`, available on CRAN
- **Webpage.** `http://stat.wharton.upenn.edu/~suw/higrad`
- **Acknowledgement.** NSF via grant CCF-1763314