Optimization geometry and implicit regularization

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Joint work with N. Srebro (TTIC), J. Lee (USC), D. Soudry (Technion), M.S. Nacson (Technion), B. Woodworth (TTIC), S. Bhojanapalli (TTIC), B. Neyshabur (TTIC-> IAS)

Optimization in ML

$h_W: x \to y$ parameterized by $\mathrm{W} \in \mathbb{R}^d$

Training data $\{(x_n, y_n): n = 1,2, \ldots N\}$

$$\widehat{W} = \underset{W}{\operatorname{argmin}} \sum_{n=1}^{N} \ell(h_W(x_n), y_n)$$

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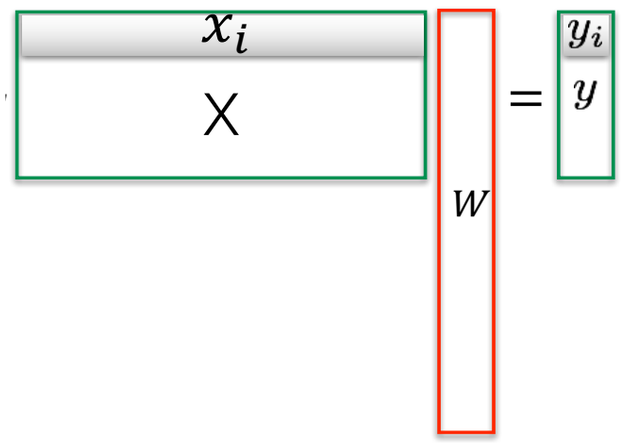

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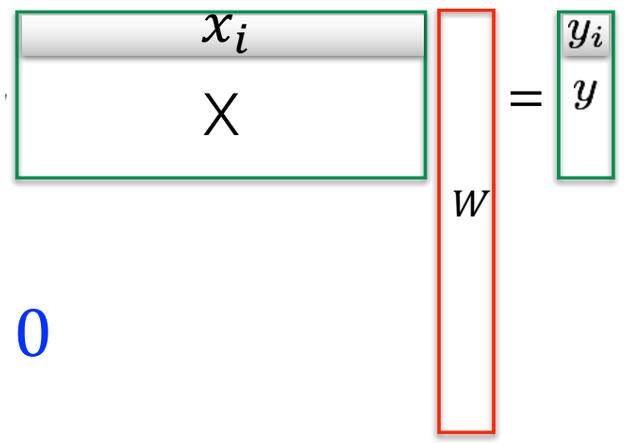

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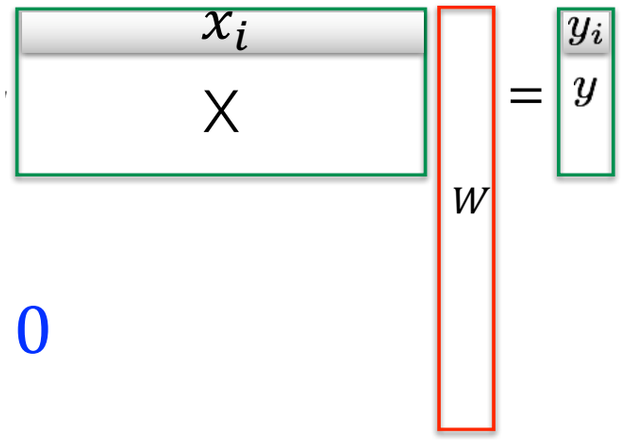

- Over parameterization: $d \gg N$
- Many global minima – all have $\sum_{n=1}^{N} \ell(h_{\widehat{W}}(x_n), y_n) = 0$
- What we really care about is $\mathbb{E}_{x,y} \ell(h_{\widehat{W}}(x), y)$

  → Different global optima have different $\mathbb{E}_{x,y} \ell(h_{\widehat{W}}(x), y)$

Learning overparameterized models

$h_W: x \to y$ parameterized by $W \in \mathbb{R}^d$

$$\widehat{W} = \underset{W}{\operatorname{argmin}} \sum_{n=1}^{N} \ell(h_W(x_n), y_n) + \mathcal{R}(W)$$

small $\mathcal{R}(\widehat{W}) \Rightarrow$

small $\mathbb{E}_{x,y}\ell(h_{\widehat{W}}(x), y)$- $\frac{1}{n}\sum_{n=1}^{N} \ell(h_{\widehat{W}}(x_n), y_n)$

Explicit regularization for
high dimensional estimation

Learning overparameterized models

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$$\widehat{W} = \underset{W}{\operatorname{argmin}} \sum_{n=1}^{N} \ell(h_W(x_n), y_n) + \cancel{\mathcal{R}(W)}$$

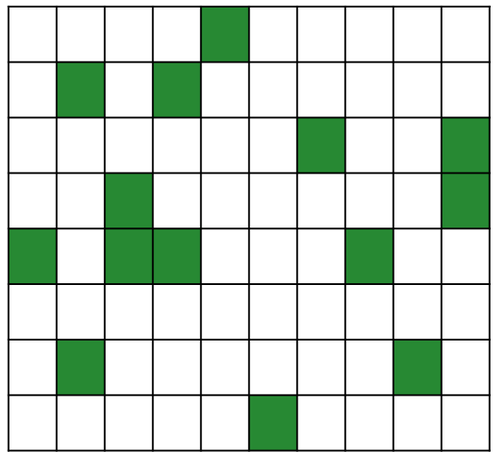
$$N \ll d$$

What happens if we don't have $\mathcal{R}(W)$?

Matrix Estimation from Linear Measurements

$$\min_{W \in \mathbb{R}^{d \times d}} L(W) := \sum_{n=1}^{N} (\langle X_n, W \rangle - y_n)^2 := \|\mathcal{X}(W) - y\|_2^2$$

e.g matrix completion, linear neural networks,…



- When $N \ll d^2$ optimization is underdetermined with

  many trivial global minima

  e.g. impute 0 or 42 or 1321234123 for matrix completion

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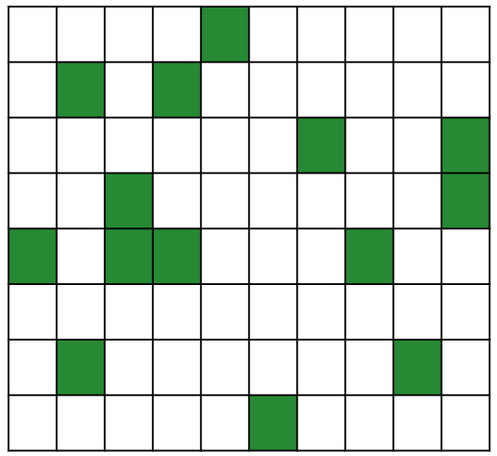

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$$\min_{U,V \in \mathbb{R}^{d \times d}} \tilde{L}(U,V) = L(UV^\top) = \|\mathcal{X}(UV^\top) - y\|_2^2$$

No explicit regularization & no rank constraint

- same trivial global minima exists

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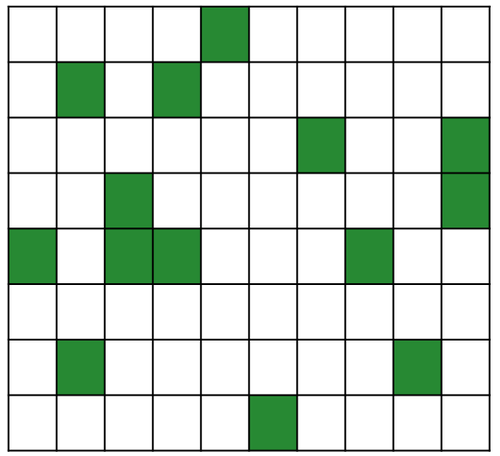

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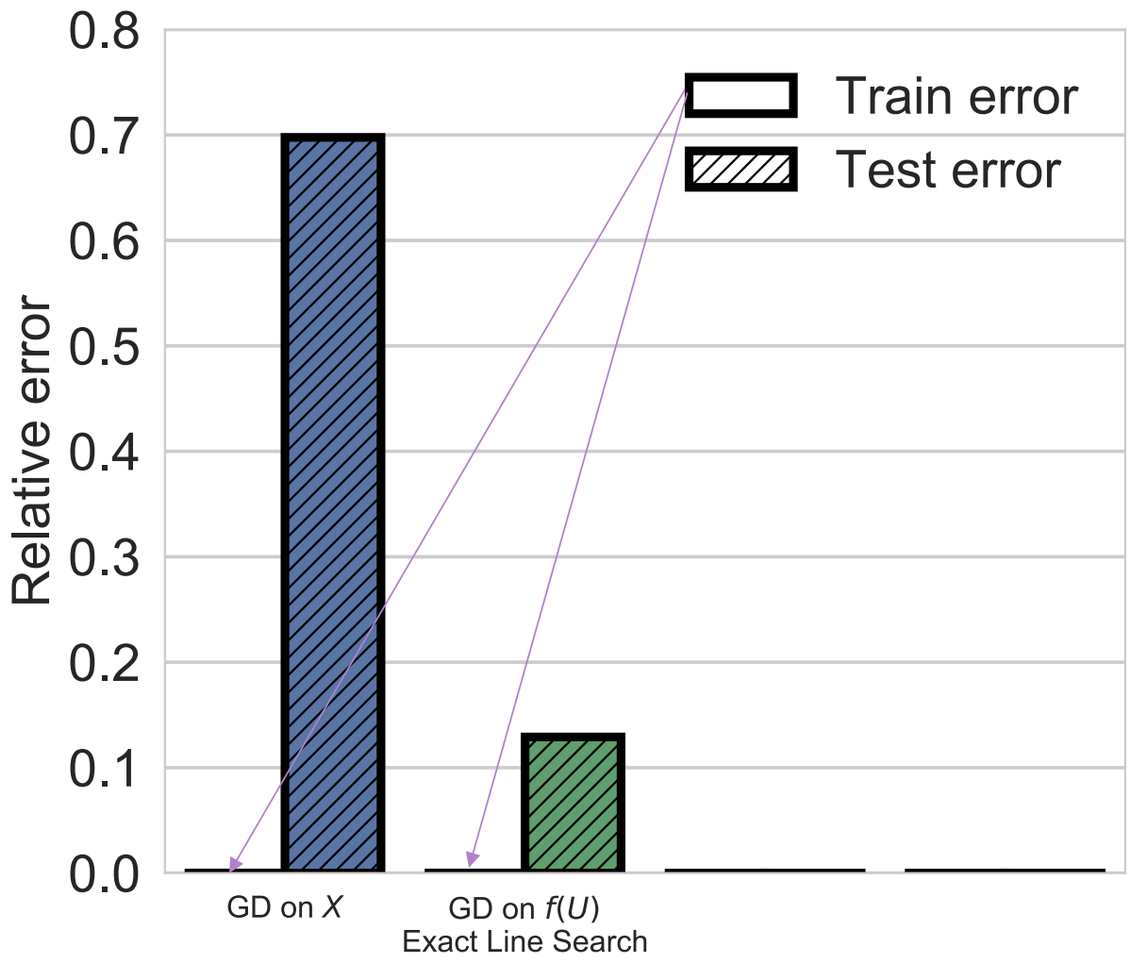
Gradient descent on $\tilde{L}(U,V)$

$$U_{k+1} = U_k - \eta\nabla_U \tilde{L}(U_k, V_k)$$
$$V_{k+1} = V_k - \eta\nabla_V \tilde{L}(U_k, V_k)$$



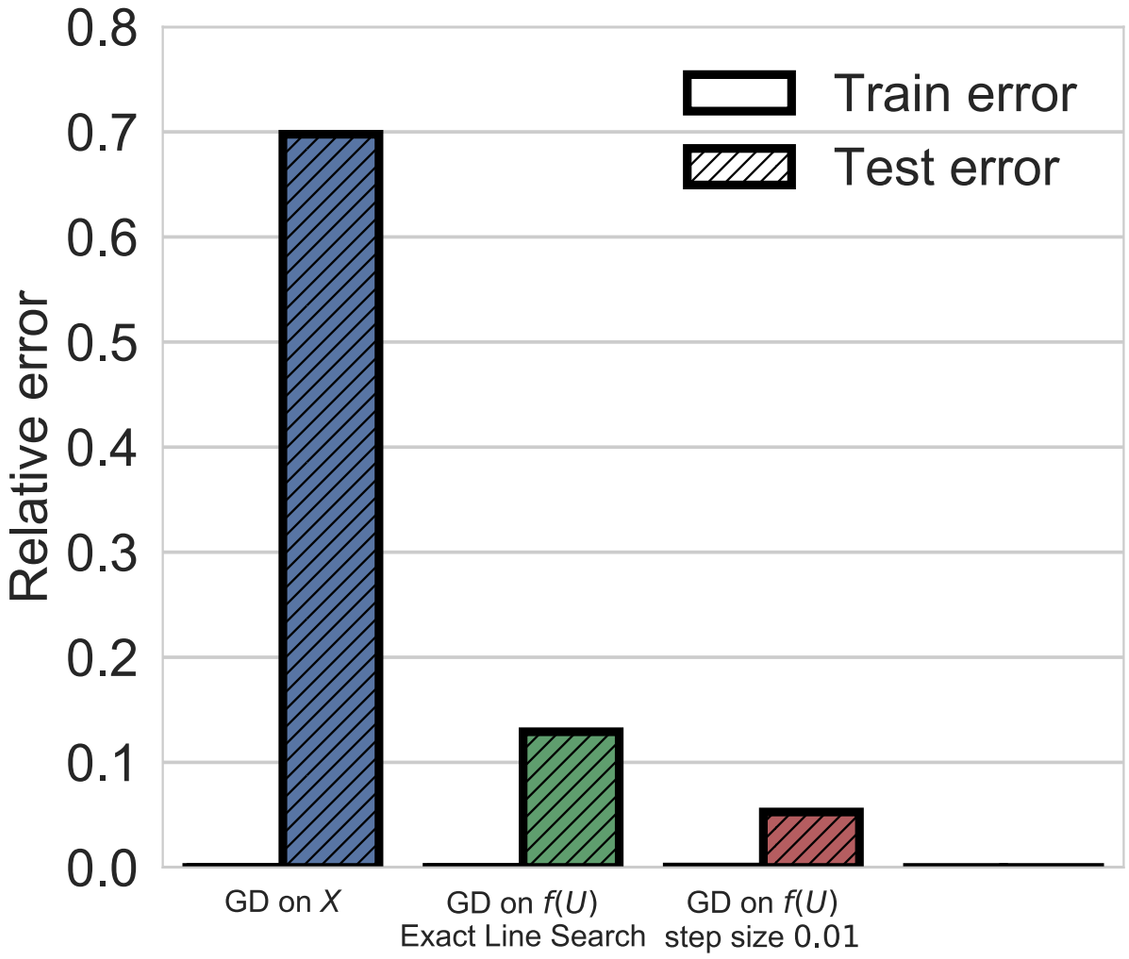
$d = 50,\ N = 300,\ X_n$ iid Gaussian, W^* rank-2 ground truth
$y = \mathcal{X}(W^*) + \mathcal{N}(0, 10^{-3})$, $y_{\text{test}} = \mathcal{X}_{\text{test}}(W^*) + \mathcal{N}(0, 10^{-3})$

$$\min_{W \in \mathbb{R}^{d \times d}} L(W) := \sum_{n=1}^{N} (\langle X_n, W \rangle - y_n)^2 := \|\mathcal{X}(W) - y\|_2^2$$

$$\min_{U,V \in \mathbb{R}^{d \times d}} \tilde{L}(U, V) = L(UV^\top) = \|\mathcal{X}(UV^\top) - y\|_2^2$$

Gradient descent on $\tilde{L}(U)$ gets to “good” global minima

G Woodworth Bhojanapalli Neyshabur Srebro, NIPS 2017



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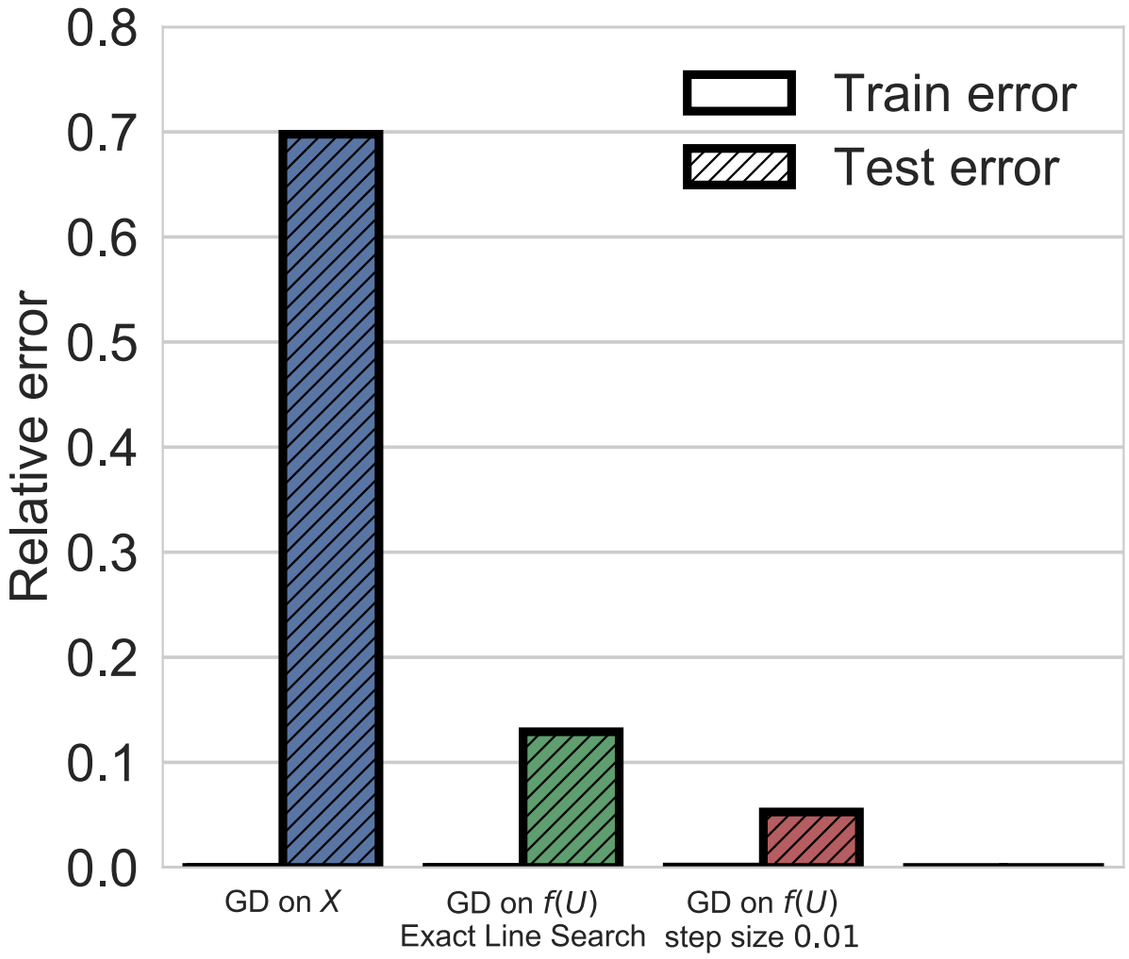
Gradient descent on $\tilde{\boldsymbol{L}}(\boldsymbol{U})$ gets to “good” global minima

Gradient descent on $\tilde{\boldsymbol{L}}(\boldsymbol{U})$ generalizes better with smaller step size

G Woodworth Bhojanapalli Neyshabur Srebro, NIPS 2017



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Question: Which global minima does gradient descent reach? Why does it generalize well?

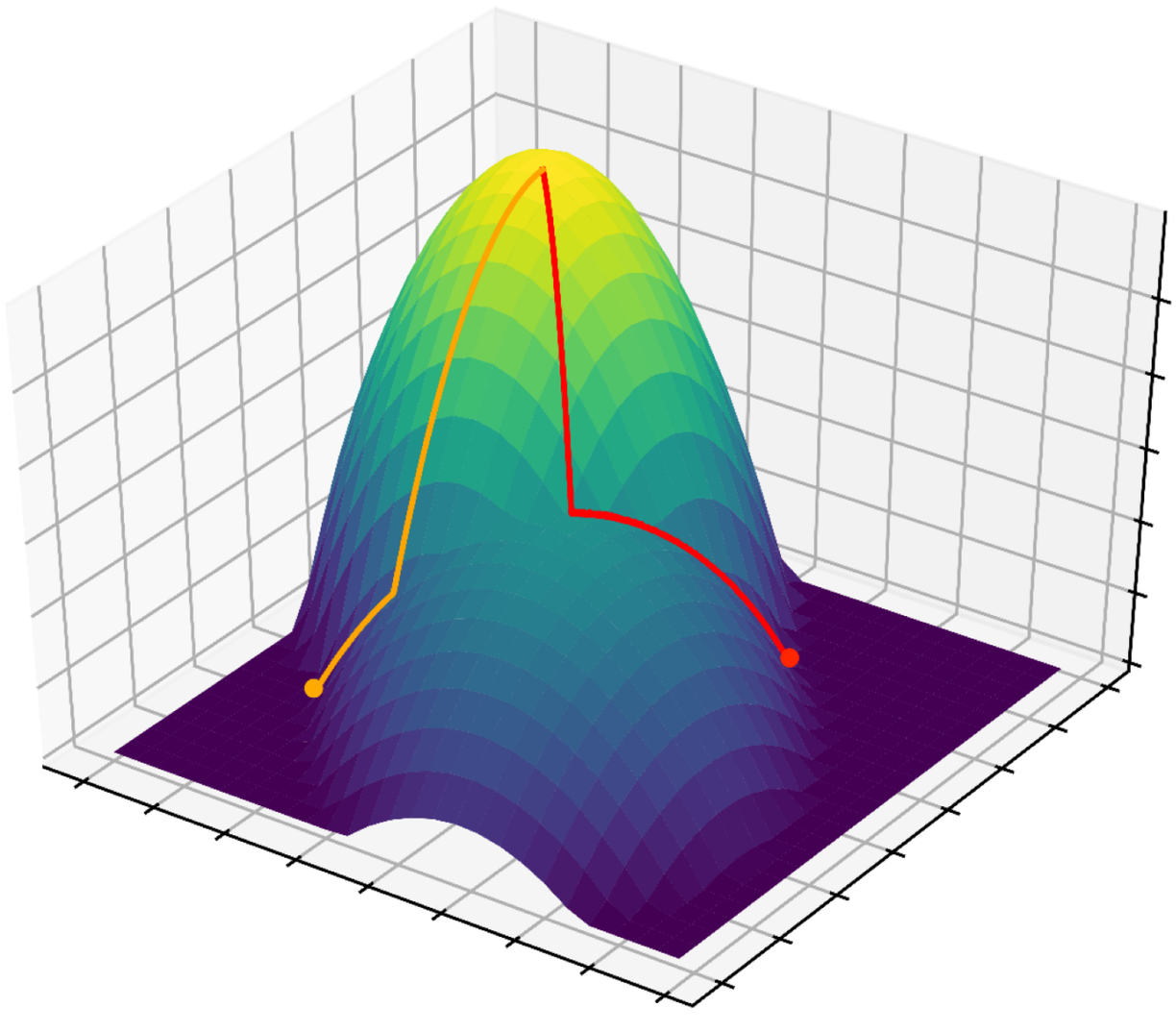
G Woodworth Bhojanapalli Neyshabur Srebro, NIPS 2017

Implicit Regularization

Different optimization algorithms

⇒ different global minimum $\widehat{W}$

⇒ different generalization $\mathbb{E}_{x,y}\ell(h_{\widehat{W}}(x), y)$



Overparameterization in neural networks

- Image datasets

  CIFAR ~ 60K images,

  ImageNet ~14M images, ~1M annotations

- Architectures for vision tasks:

  AlexNet (2012): 8 layers, 60M parameters

  VGG-16 (2014): 16 layers, 138M parameters

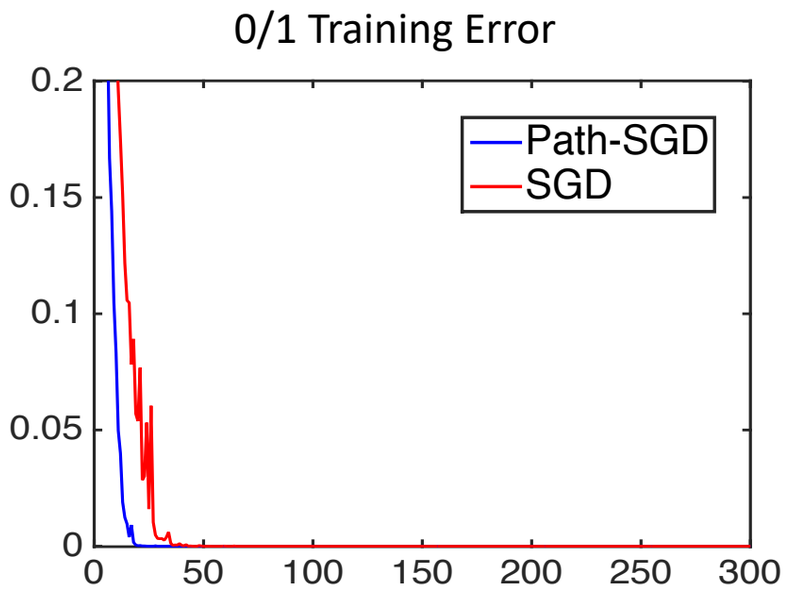
  ResNet (2015): 152 layers, …

NNs trained using local search have good generalization even without explicit regularization or early stopping

(Neyshabur et al. 2014, Zhang et al. 2016, Hoffer et al. 2017)

Bias of optimization algorithms

- Effect of optimization geometry (Neyshabur et al. 2015)



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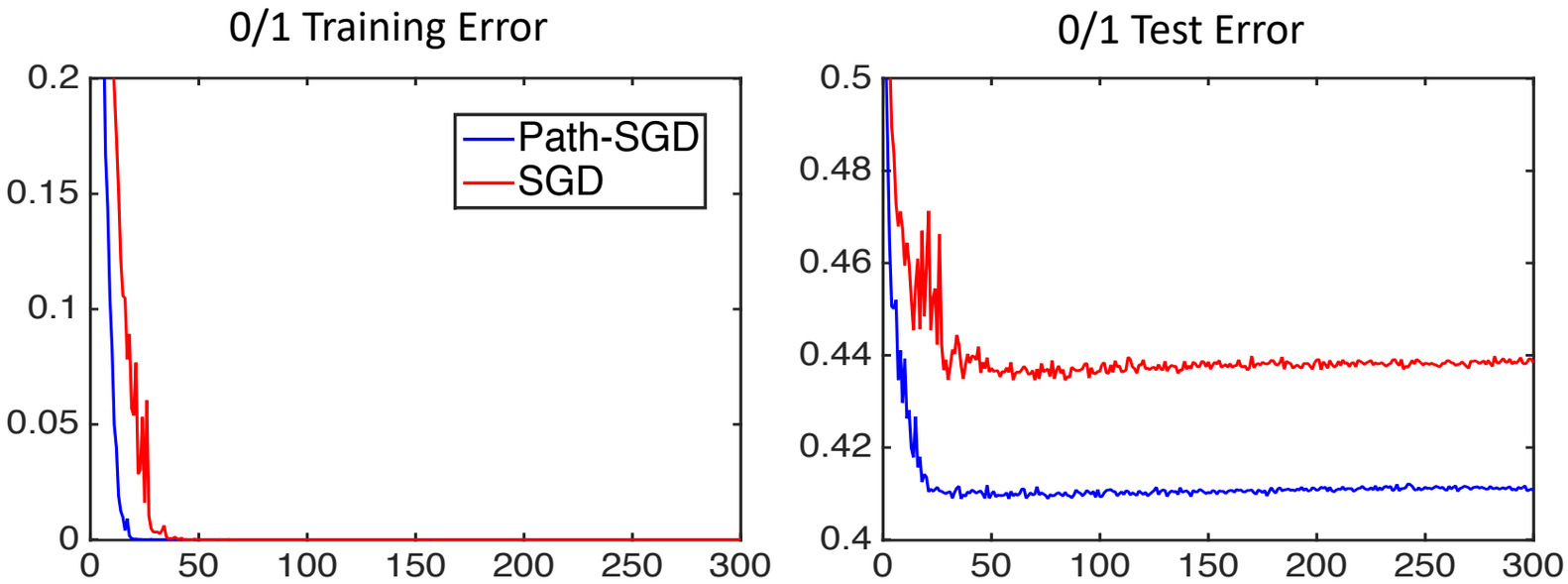

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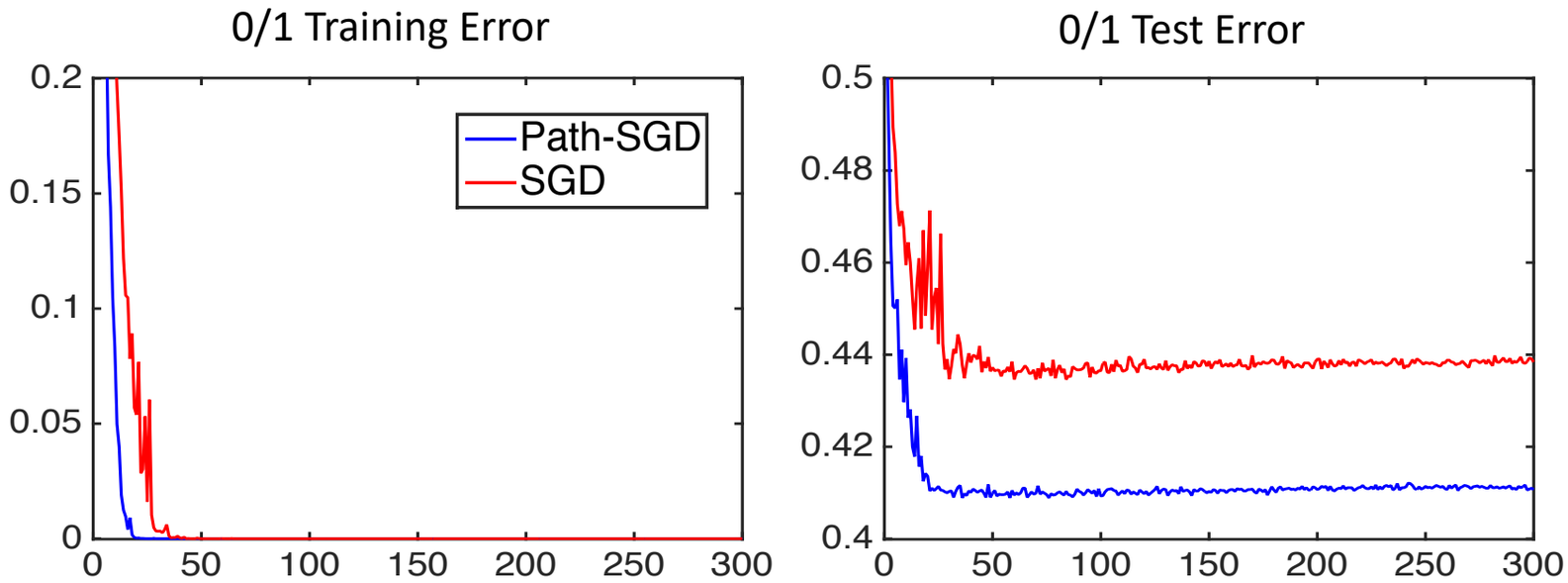

- Effect of size of minibatch (Keskar et al. 2017,Dihn et al. 2017)
- Effect of adaptive algorithms (Wilson et al. 2017)
- Learning to learn (Abdrychowicz et al. 2016, Finn et al . 2017)

Implicit Regularization

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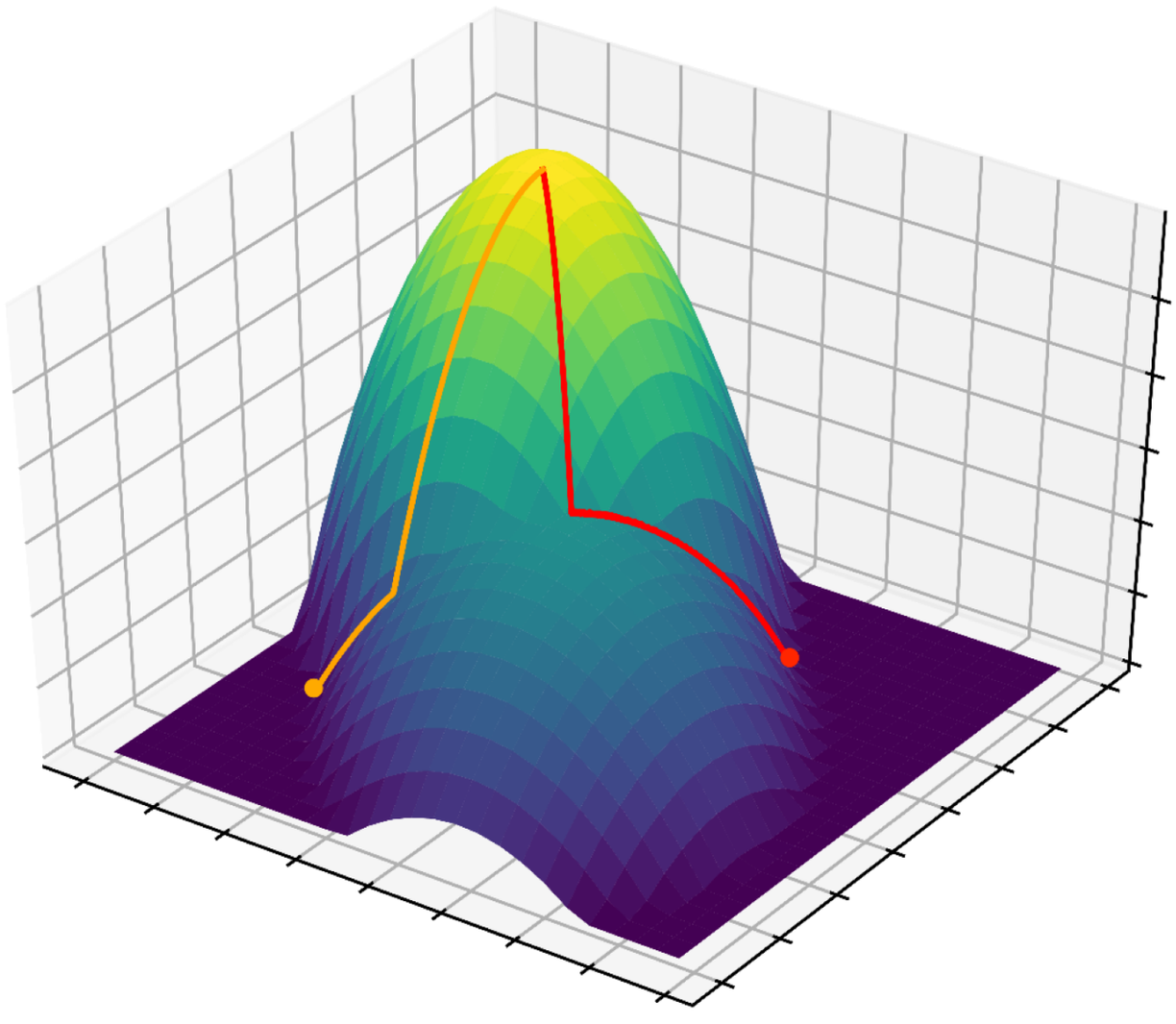

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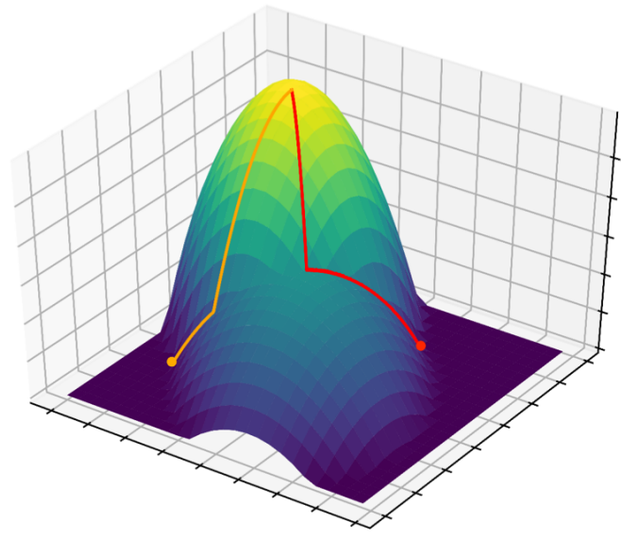
How does this depend on optimization geometry, initialization, step size, momentum, stochasticity?



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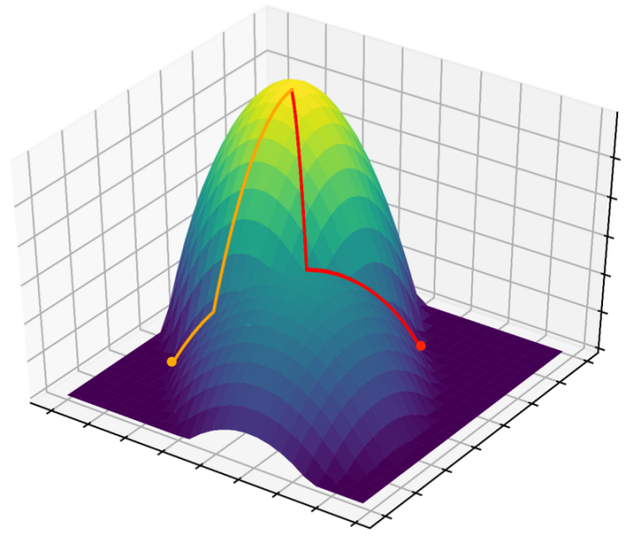
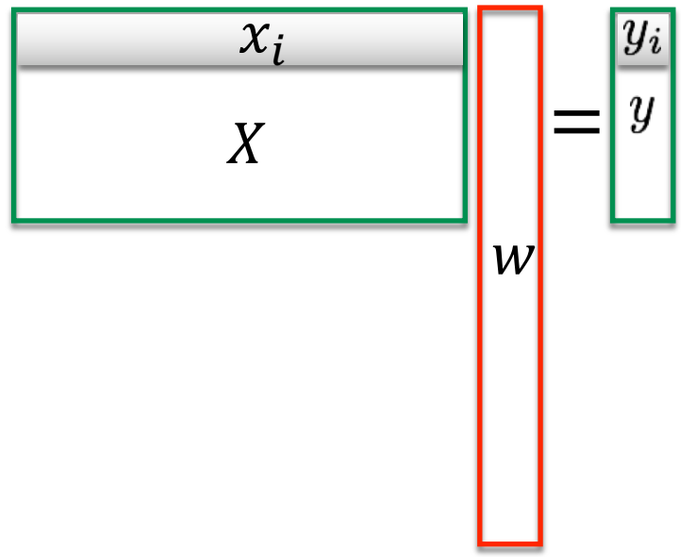


Understanding the implicit bias could enable

- Optimization algorithms for faster convergence AND better generalization
- New regularization techniques
- Efficiently train smaller networks

Gradient descent: linear regression

$$\min_w L(w) = \sum_{n=1}^{N} (\langle x_n, w \rangle - y_n)^2$$



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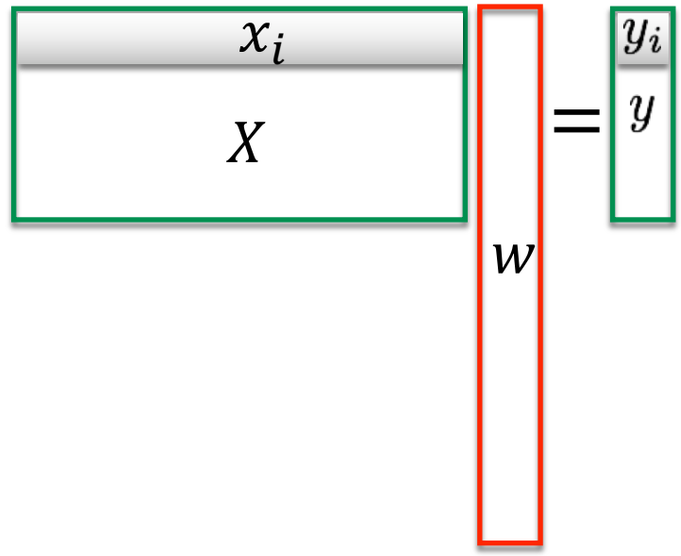

Gradient descent initialized at $w(0)$

$$w(t+1) = w(t) - \eta \nabla_w L(w(t))$$

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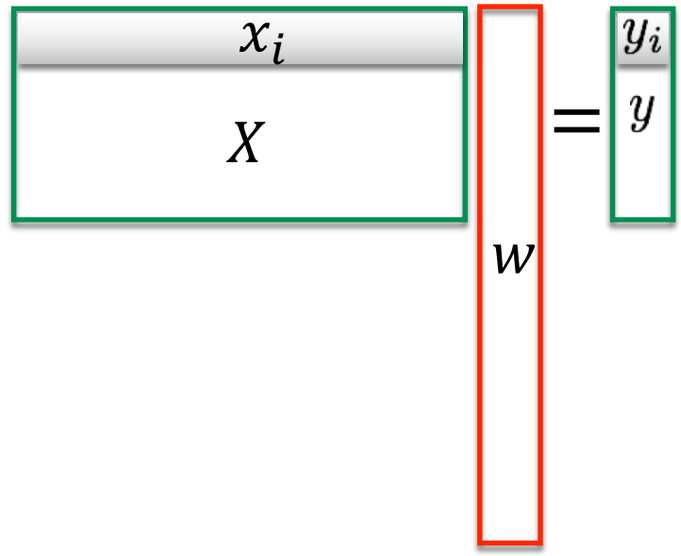

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$$w(t) \to \underset{Xw=y}{\text{argmin}} \|w\|_2$$

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Independent of step size η, momentum, instancewise stochastic gradient descent

Gradient descent: linear regression

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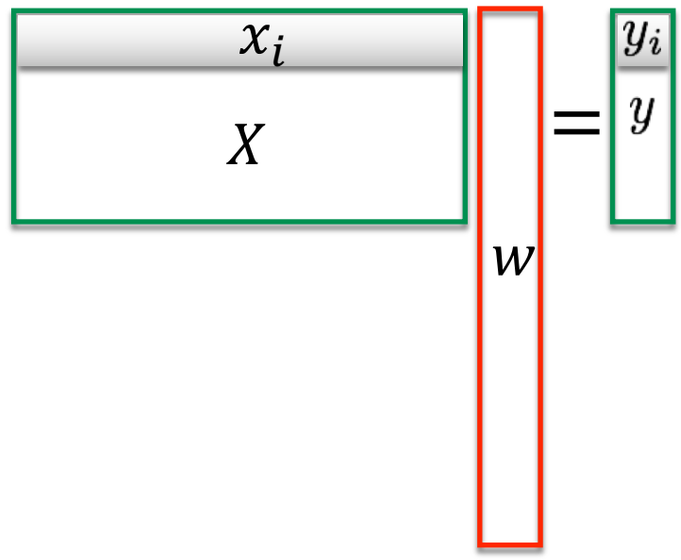

Gradient descent initialized at $w(0)$

$$w(t+1) - w(t) - \eta \nabla_w L(w(t))$$

$$\nabla_w L(w(t)) = \sum_{n=1}^{N} (\langle x_n, w(t) \rangle - y_n) x_n$$

Updates lie on a low dimensional affine manifold

$$\Delta w(t) \in \text{span}(x_n)$$

$$\widehat{w}_{(s)gd} = \underset{Xw=y}{\text{argmin}} \|w - w(0)\|_2$$

Same argument for linear models $\hat{y}(x) = \langle w, x \rangle$ and loss functions $\ell(\hat{y}(x), y)$ with unique finite root at $\hat{y} = y$

Can we get such results for other problems and other optimization algorithms?

First, same problem different optimization algorithms

Mirror descent w.r.t potential ψ

Gradient descent

$$w(t+1) = \operatorname*{argmin}_{w} \eta\langle w, \nabla_w L(w(t)) + \frac{1}{2}\|w - w(t)\|_2^2$$

Mirror descent w.r.t potential ψ

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Mirror Descent w.r.t. strongly convex potential ψ

$$w(t+1) = \underset{w}{\text{argmin}}\ \eta\langle w, \nabla_w L(w(t)) + D_\psi\left(w, w(t)\right)$$

$$D_\psi\left(w, w(t)\right) = \psi(w) - \psi(w(t)) - \langle \nabla\psi(w(t), w - w(t)\rangle$$

$$e.g.\ \psi(w) = \textstyle\sum_i w[i] \log w[i] \rightarrow D_\psi\big(w, w(t)\big) = KL(w, w(t))$$

Mirror descent w.r.t potential ψ

$$w(t+1) = \underset{w}{\text{argmin}}\ \eta\langle w, \nabla_w L(w(t)) + D_\psi\left(w, w(t)\right)$$

$$\nabla\psi(w(t+1)) = \nabla\psi(w(t)) - \sum_{n=1}^{N} \ell'(w(t))x_n$$

G, Lee, Soudry, Srebro. Arxiv 2018

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Dual updates lie on the low dimensional affine manifold $\Delta w(t) \in \text{span}(x_n)$

If $\nabla\psi\left(w(0)\right) = 0$

$w(t) \to \underset{Xw=y}{\text{argmin}}\ \psi(w)$

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$$w(t) \to \underset{Xw=y}{\text{argmin}}\ D_\psi(w, w(0))$$

- Again independent of step size, stochasticity, dual momentum
- Also works with affine constraints on w

  Exponentiated gradient descent

  → implicit entropic regularization $\psi(w) = \sum_i w[i]\log(w[i])$

G, Lee, Soudry, Srebro. Arxiv 2018

Steepest descent w.r.t. norm $\|.\|$

Gradient descent

$$w(t+1) = w(t) + \eta \Delta w(t)$$

$$\Delta w(t) = \underset{v:\|v\|_2 \leq 1}{\text{argmin}} \ \langle v, \nabla_w L(w(t)) \rangle$$

Steepest Descent w.r.t. general norm $\|.\|$

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$$\Delta w(t) = \underset{v:\|v\| \leq 1}{\text{argmin}} \ \langle v, \nabla_w L(w(t)) \rangle$$

e.g. Coordinate descent $\|.\| = \|.\|_1$

G, Lee, Soudry, Srebro. Arxiv 2018

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$$w(t) \overset{?}{\to} \text{argmin}_{Xw=y} \ \|w - w(0)\|$$

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Steepest descent w.r.t. norm $\|.\|$

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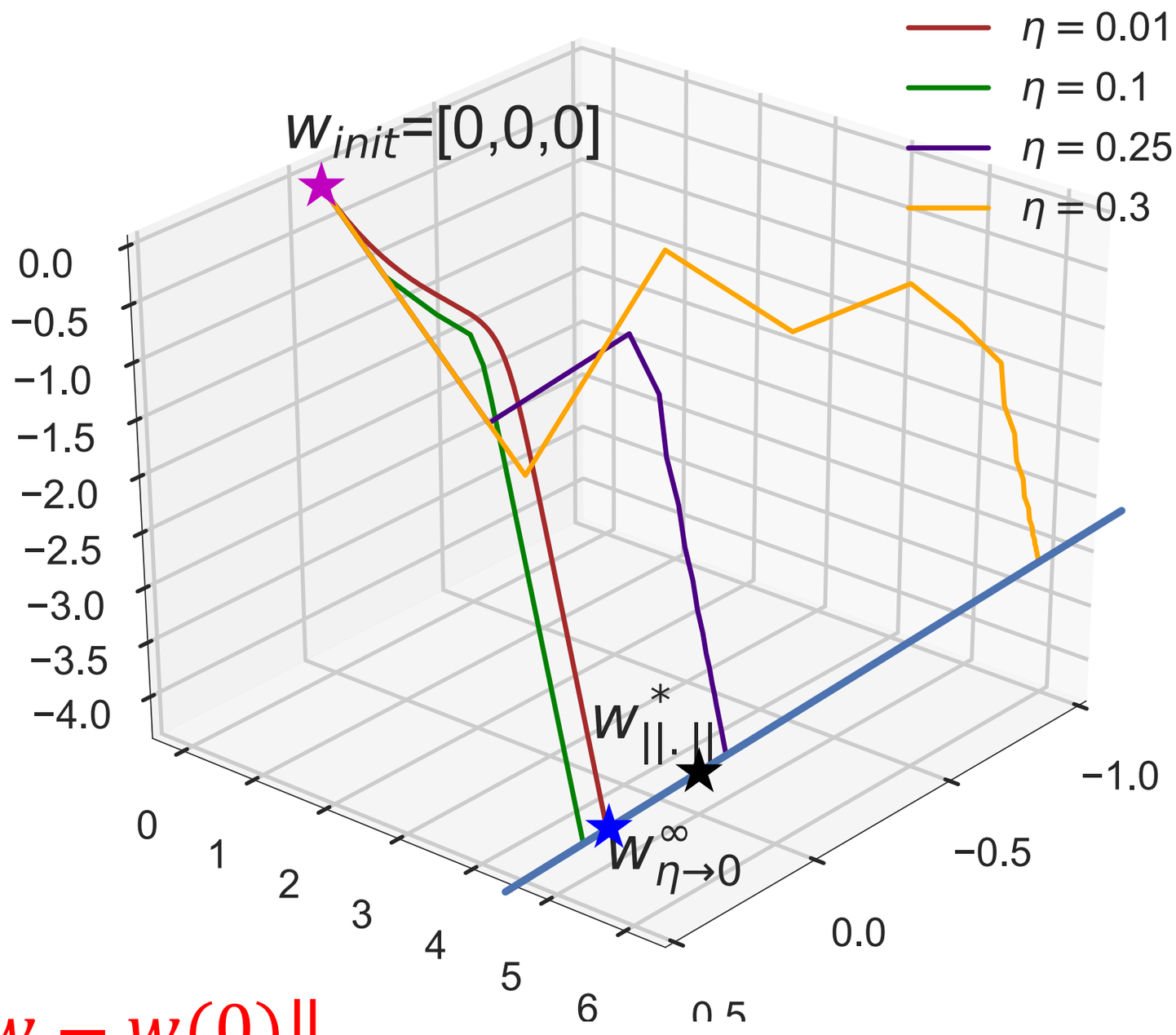

Even for $\eta \to 0$:

$w(t) \nrightarrow \text{argmin}_{Xw=y} \|w - w(0)\|$

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Can we get such results for other problems and other optimization algorithms?

How about gradient descent on other problems or different parameterizations?

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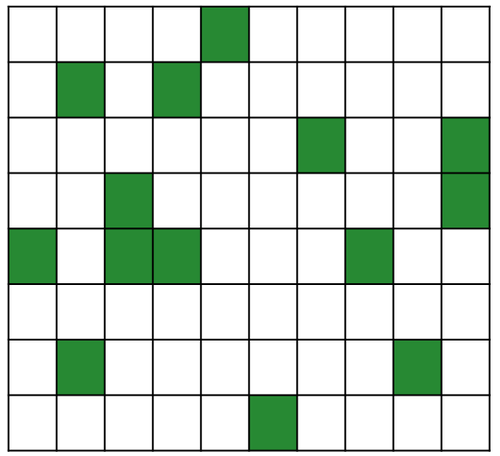
$$\min_{W\in\mathbb{R}^{d\times d}} L(W) := \sum_{n=1}^{N}(\langle X_n, W\rangle - y_n)^2 := \|\mathcal{X}(W) - y\|_2^2$$

e.g matrix completion, linear neural networks,…



- When $N \ll d^2$ optimization is underdetermined with

  many trivial global minima

  e.g. impute 0 or 42 or 1321234123 for matrix completion

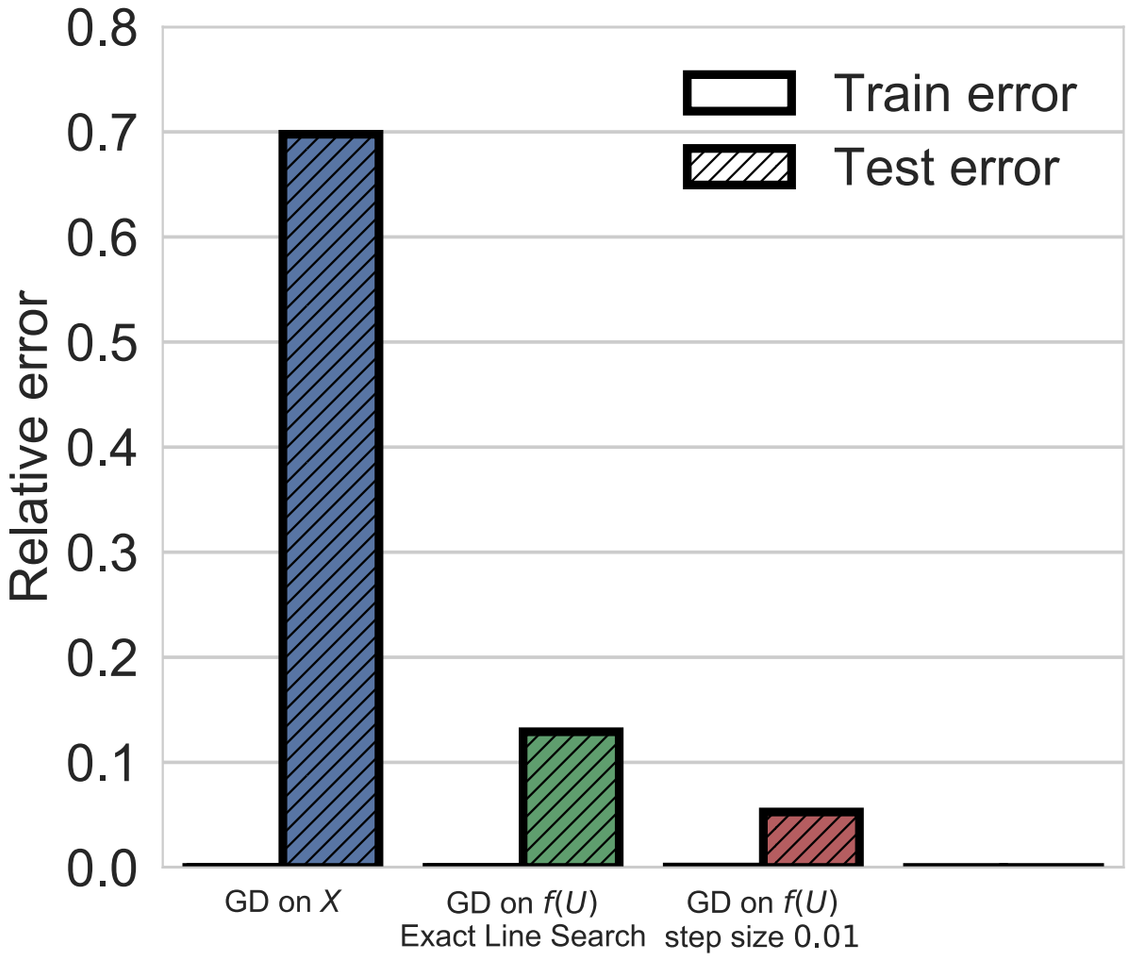
$$\min_{U,V\in\mathbb{R}^{d\times d}} \tilde{L}(U,V) = L(UV^\top) = \|\mathcal{X}(UV^\top) - y\|_2^2$$

No explicit regularization & no rank constraint

- same trivial global minima exists

Gradient descent on $\tilde{L}(U,V)$

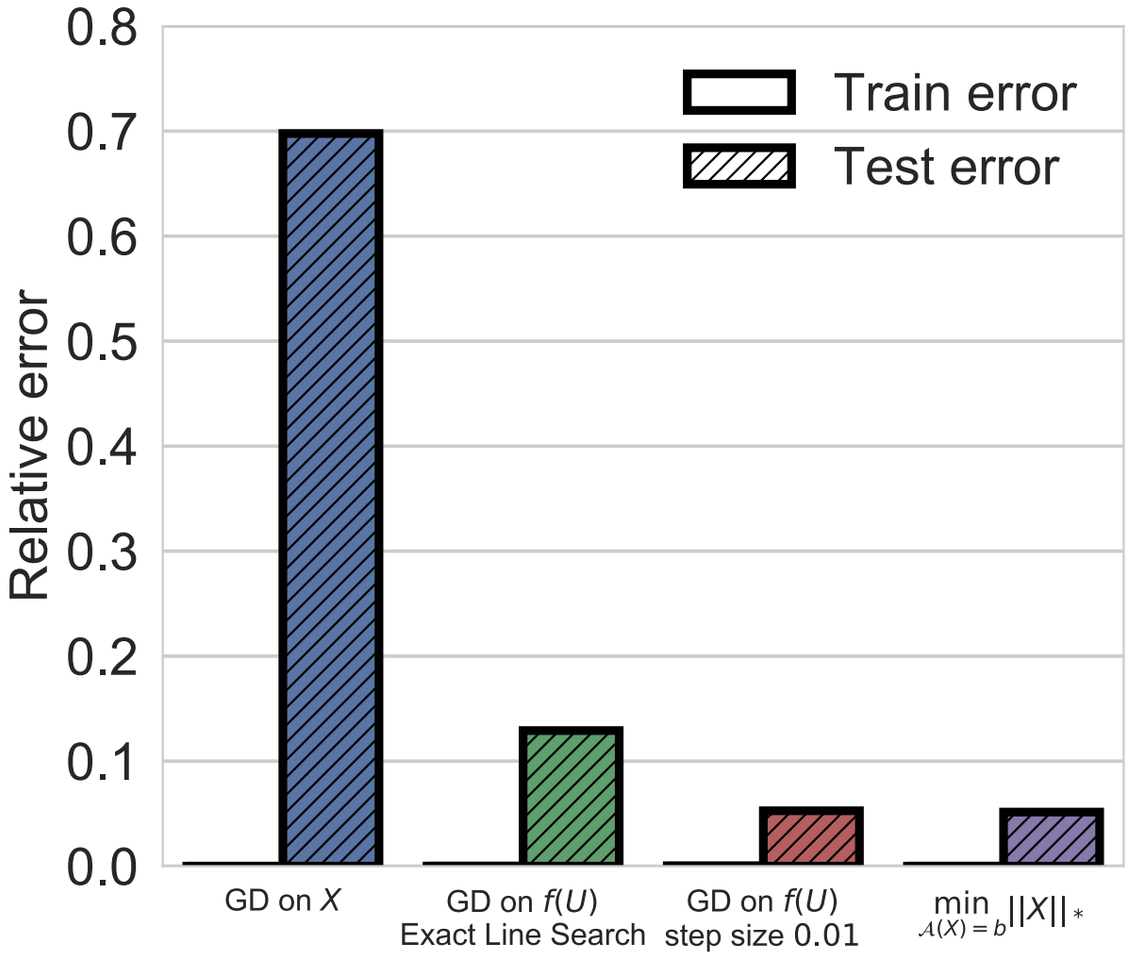
$$U_{k+1} = U_k - \eta\nabla_U \tilde{L}(U_k, V_k)$$
$$V_{k+1} = V_k - \eta\nabla_V \tilde{L}(U_k, V_k)$$

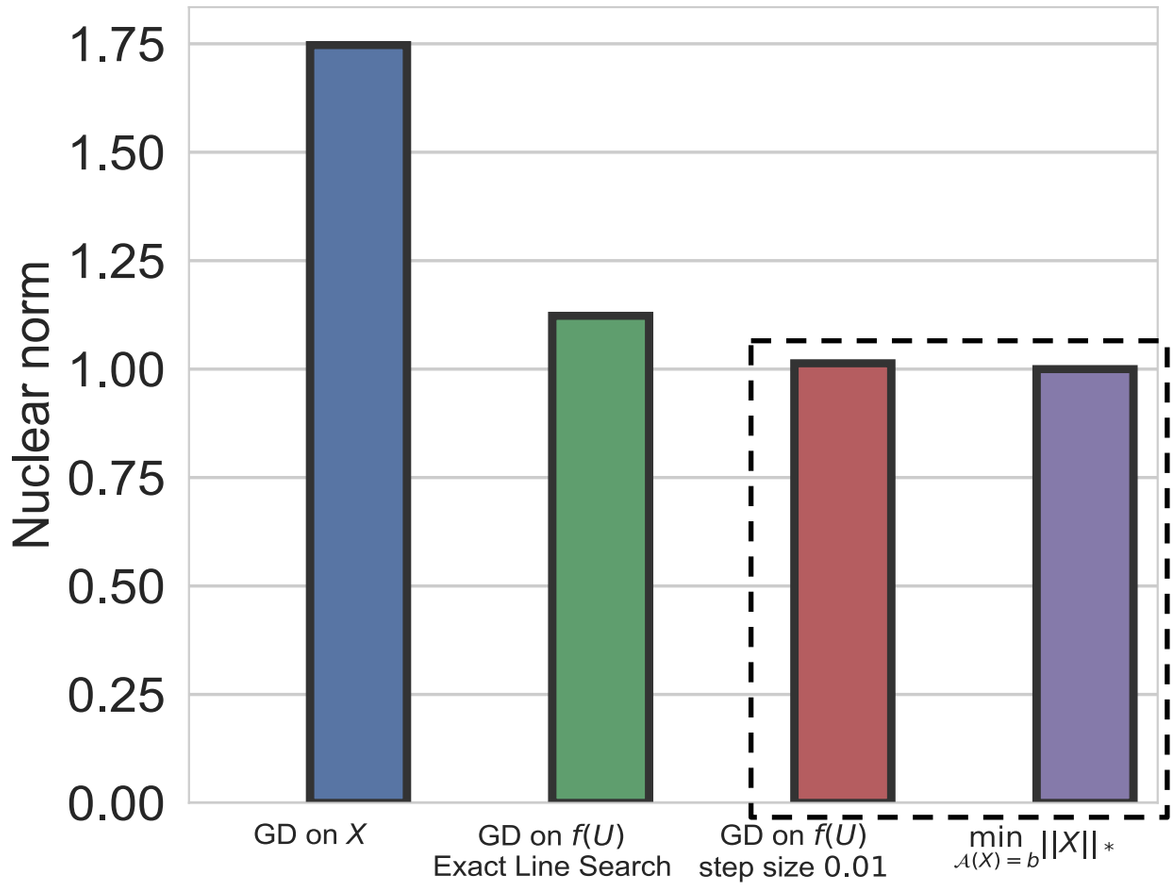


$d = 50,\ N = 300,\ X_n$ iid Gaussian, W^* rank-2 ground truth
$y = \mathcal{X}(W^*) + \mathcal{N}(0, 10^{-3})$, $y_{\text{test}} = \mathcal{X}_{\text{test}}(W^*) + \mathcal{N}(0, 10^{-3})$

Question: Which global minima does gradient descent reach? Why does it generalize well?

G Woodworth Bhojanapalli Neyshabur Srebro, NIPS 2017





Gradient descent on $\tilde{L}(U)$ converges to a minimum nuclear norm solution

G Woodworth Bhojanapalli Neyshabur Srebro, NIPS 2017

Conjecture (informal)

Gradient descent on $\tilde{L}(U,V)$ converges to the minimum nuclear norm solution

$$W(t) = U(t)V(t)^\top \to W^*_{\mathrm{NN}} = \operatorname*{argmin}_{\mathcal{X}(W)=y} \|W\|_*$$

when,

- Initialization is close to 0
- Step size is very small → $\dot{U}_t = \frac{\mathrm{d}U_t}{\mathrm{d}t} = -\nabla_U \tilde{L}(U)$

G Woodworth Bhojanapalli Neyshabur Srebro, NIPS 2017

Commutative X_i

$$X_i X_j = X_j X_i \text{ for all } i,j \in [N]$$

$$W(t) = e^{\mathcal{X}^*(s_t)}\, W(0)\, e^{-\mathcal{X}^*(s_t)} \text{ for some } s_t \in \mathbb{R}^N$$

$\eta \to 0$ necessary to remain in the (non-linear) manifold

G Woodworth Bhojanapalli Neyshabur Srebro, NIPS 2017

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$\eta \to 0$ necessary to remain in the (non-linear) manifold

Let $U_\infty(\alpha)$ be the solution of gradient flow initialized at $U_0 = \alpha I$.
If measurements X_n commute, i.e. $X_i X_j = X_j X_i$, and
if $\bar{W}_\infty = \lim_{\alpha \to 0} U_\infty(\alpha) U_\infty(\alpha)^\top$ exists and satisfies $L(\bar{W}_\infty) = 0$, then

$$\bar{W}_\infty = W^*_{\mathrm{NN}} = \min_{\mathcal{X}(W)=y} \|W\|_*$$

Conjecture proved for RIP X_n by Li et al. (2018)

G Woodworth Bhojanapalli Neyshabur Srebro, NIPS 2017

Proof Ideas

- Characterize the manifold in which the $w(t)$ lie on

  → $w(0) + span(x_n)$ for gradient descent

  → $\nabla\psi^{-1}\left(\nabla\psi\left(w(0)\right) + span(x_n)\right)$ for mirror descent

  → $e^{X^*(s)}W(0)e^{X^*(s)}$ for matrix factorization with $\eta \to 0, \|W(0)\| \to 0$, commutative X_n

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  → $e^{\mathcal{X}^*(s)}W(0)e^{\mathcal{X}^*(s)}$ for matrix factorization with $\eta \to 0, \|W(0)\| \to 0$, commutative X_n

- Show that all the global minima on the manifold satisfy the KKT conditions for "regularized" problem
  → $\min_{\mathrm{Xw=y}} \|w - w(0)\|_2$
  → $\min_{Xw=y} D_\psi\left(w, w(0)\right)$
  → $\min_{\mathcal{X}(W)=y} \|W\|_*$

Losses with a unique finite root

- Robust characterization of for general mirror descent with potential ψ

$$w(t) \to \min_{Xw=y} D_\psi(w, w(0))$$

- No useful characterization for generic steepest descent w.r.t norm $\|.\|$
  → even when $\|.\|^2$ strongly convex
  → even for $\eta \to 0$

- Fragile characterization for matrix factorization

$$W(t) \to \min_{W \succcurlyeq 0,\, \mathcal{X}(W)=y} \|W\|_*$$

  → ONLY for $\|W(0)\| \to 0, \eta \to 0$
  → Proven only for RIP measurements
  → initialization close to 0 is particularly bad!!

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What happens with other losses?

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What happens with other losses?

→ Very different for logistic regression – no finite minima

Implicit bias when global minimum is unattainable!

Logistic regression on separable data

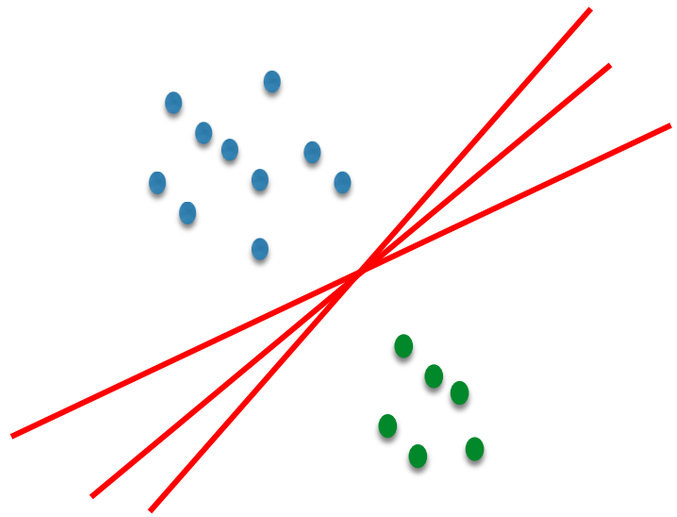
Gradient descent: logistic regression

$$\min_w L(w) = \sum_{n=1}^{N} \log(1 + \exp(-y_n \langle x_n, w \rangle))$$

Gradient descent initialized at $w(0)$

$$w(t+1) = w(t) - \eta \nabla_w L(w(t))$$

$$\nabla_w L(w(t)) = \sum_{n=1}^{N} r_n(t) x_n$$



Soudry, Hoffer, Srebro, ICLR 2018

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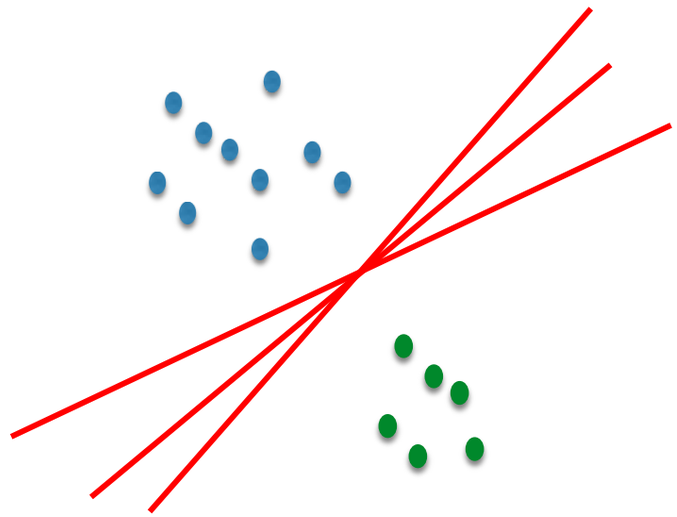

$$\nabla_w L(w(t)) = \sum_{n=1}^{N} r_n(t) x_n$$

but $\|w(t)\| \to \infty$!

Soudry, Hoffer, Srebro, ICLR 2018

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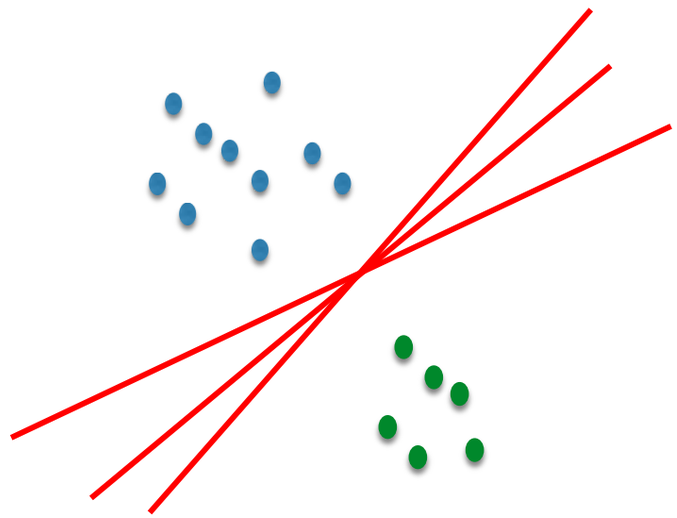

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$$\frac{w(t)}{\|w(t)\|_2} \to \operatorname*{argmax}_{w:\|w\|_2 \le 1} \min_n y_n \langle w, x_n \rangle$$

Independent of step size $\boldsymbol{\eta}$ and initialization $\boldsymbol{w(0)}$

Soudry, Hoffer, Srebro, ICLR 2018

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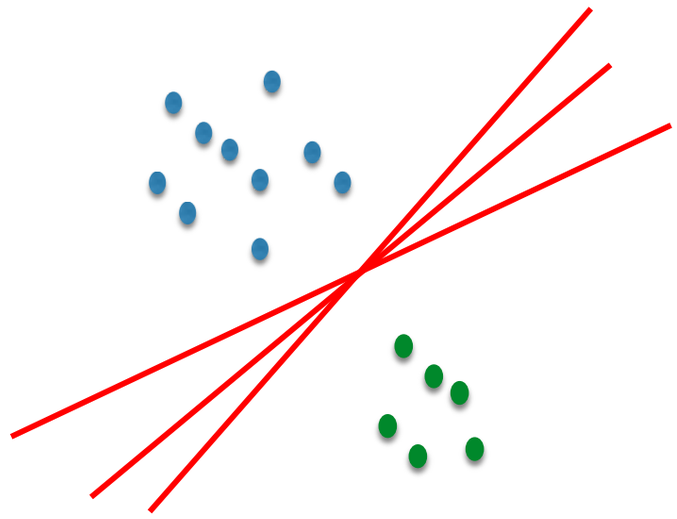

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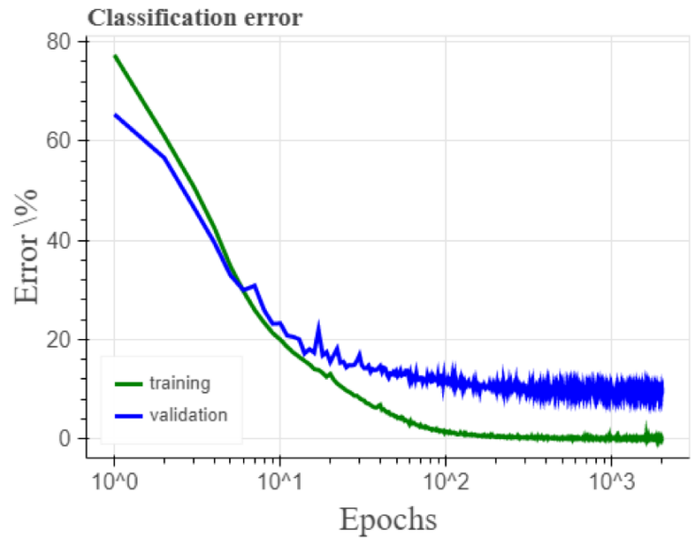
Holds for linear classifiers $\hat{y}(x) = \langle w, x \rangle$ and any strictly monotone loss $\ell(\hat{y}(x), y)$ with exponential tail

Soudry, Hoffer, Srebro, ICLR 2018

How fast is the margin maximized?

Fixed step size η

- $O\left(\frac{1}{\log(t)}\right)$ - extremely slow!!
- Compare with $O\left(\frac{1}{t}\right)$ convergence of $L(w)$



Soudry, Hoffer, Srebro, 2018

Schpiegel, Lee, **G**, Srebro, Soudry, Arxiv 2018

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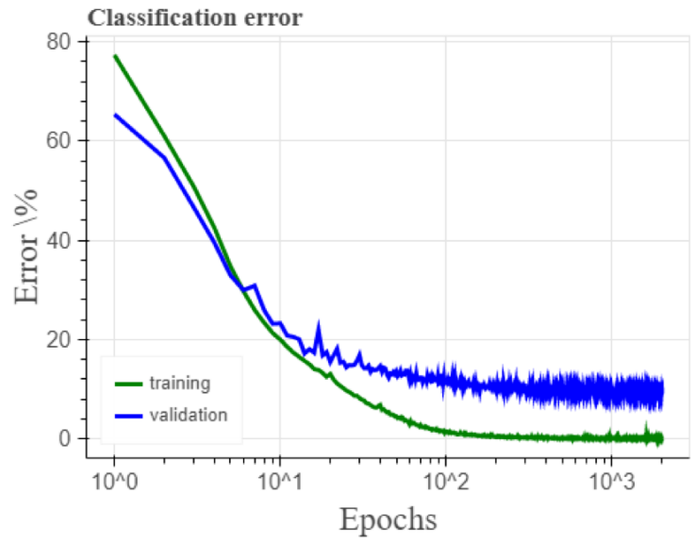

Soudry, Hoffer, Srebro, 2018

Can we use lighter or heavier tail to get faster convergence?

No. exponential-tail yields optimal rate.

- For $\ell(u) = \exp(-u^\nu), \nu > 1$, margin converges as $O\left(\frac{1}{\log^{1/\nu} t}\right)$
- For $\ell(u) = \exp(-u^\nu), \frac{1}{4} \leq \nu < 1$, margin converges as $\frac{C}{\nu \log t}$
- For $\ell(u) \propto u^{-\nu}$, does **not** converge to max-margin

Schpiegel, Lee, **G**, Srebro, Soudry, Arxiv 2018

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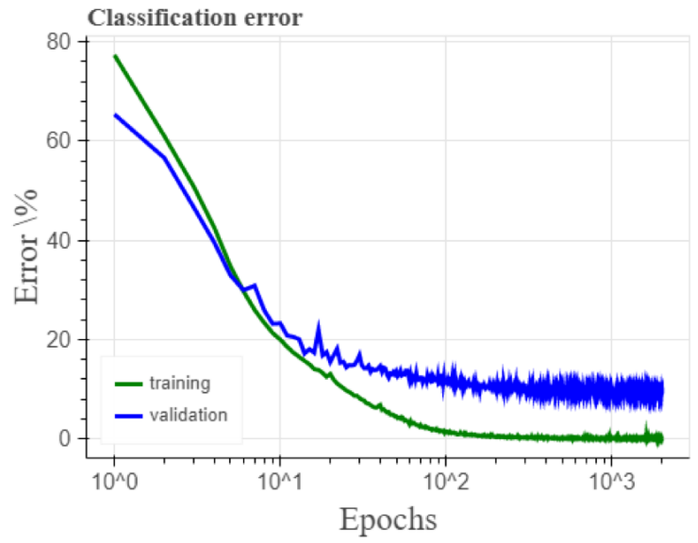

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Any other way to get faster convergence?

Yes. Stepsize $\eta \propto 1/\|\nabla\mathcal{L}\|$ yield $\tilde{O}\left(\frac{1}{\sqrt{t}}\right)$ convergence

(comparable to best hard-margin SVM algorithms)

Schpiegel, Lee, **G**, Srebro, Soudry, Arxiv 2018

Implicit bias on strictly monotone losses with exponential tail

Can we get a more robust characterization compared to regression-type losses?

Steepest descent w.r.t. norm $\|.\|$

$$w(t+1) = w(t) + \eta \Delta w(t)$$

$$\Delta w(t) = \underset{v:\|v\| \leq 1}{\text{argmin}} \ \langle v, \nabla_w L(w(t)) \rangle$$

G, Lee, Soudry, Srebro. Arxiv 2018

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$$\frac{w(t)}{\|w(t)\|} \to \max_{w:\|w\|\leq 1} \min_n y_n \langle w, x_n \rangle$$

→ Independent of initialization

→ Small enough η

G, Lee, Soudry, Srebro. Arxiv 2018

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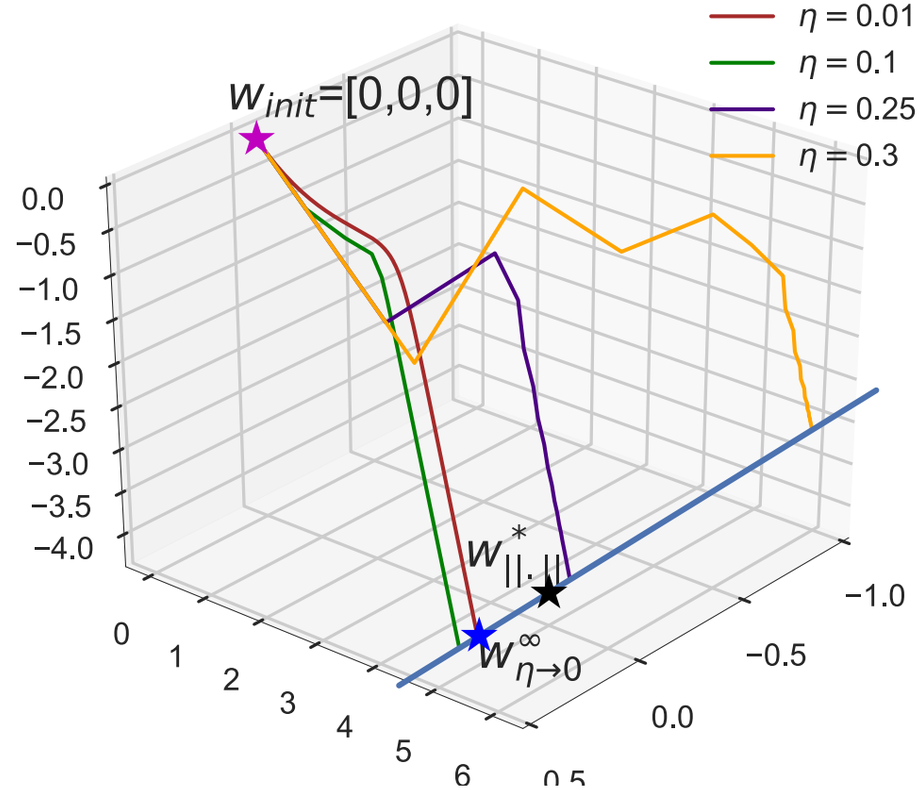
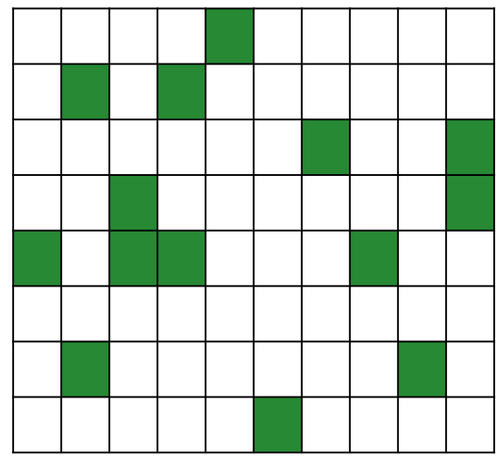
Compare with squared loss →



G, Lee, Soudry, Srebro. Arxiv 2018

Matrix Estimation from Linear Measurements

e.g matrix completion, linear neural networks,…



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  e.g. impute 0 or 42 or 1321234123 for matrix completion

Gradient descent on $L(U,V)$

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G, Lee, Soudry, Srebro. Arxiv 2018

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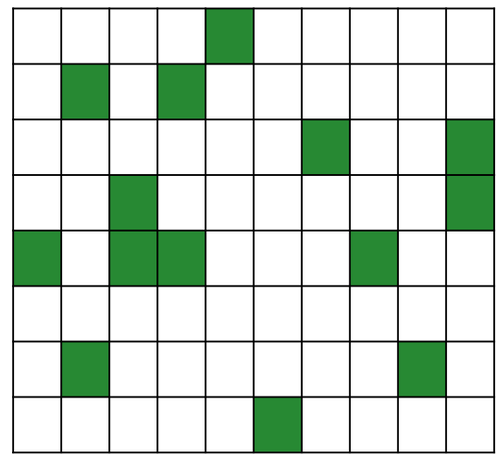

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Let $W(t) = U(t)U(t)^\top$. For any full rank $W(0)$ and any η_t such that $\{L(W(t))\}_t$ is strictly decreasing, if $\frac{\Delta W(t)}{\|\Delta W(t)\|}$ and $\frac{\nabla L(W(t))}{\|\nabla L(W(t))\|}$ exists, then

$$\frac{W(t)}{\|W(t)\|_*} \to \max_{\|W\|_* \le 1} \min_n y_n \langle X_n, W \rangle$$

G, Lee, Soudry, Srebro. Arxiv 2018

Strictly monotone losses

- Gradient descent

$$\frac{w(t)}{\|w(t)\|_2} \to \max_{\|w\|_2 \le 1} \min_n y_n \langle x_n, w \rangle$$

→ Independent of initialization
→ Any step size leading to descent algorithm

- Steepest descent w.r.t norm $\|.\|$

$$\frac{w(t)}{\|w(t)\|} \to \max_{\|w\| \le 1} \min_n y_n \langle x_n, w \rangle$$

→ Independent of initialization
→ Any step size leading to descent algorithm

- Matrix factorization

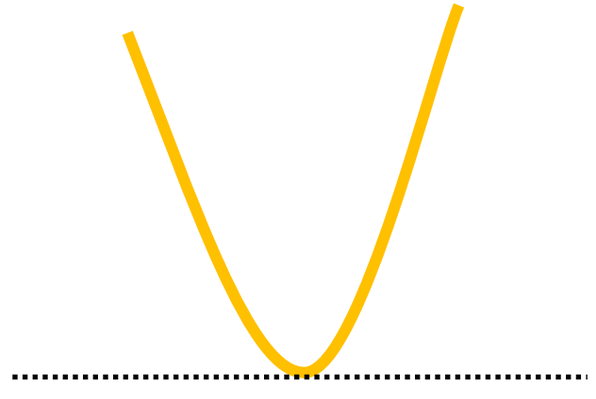
$$\frac{W(t)}{\|W(t)\|_*} \to \max_{\|W\|_* \le 1} \min_n y_n \langle X_n, W \rangle$$

→ Independent of initialization
→ Any step size leading to descent algorithm

Simplicity from Asymptotics

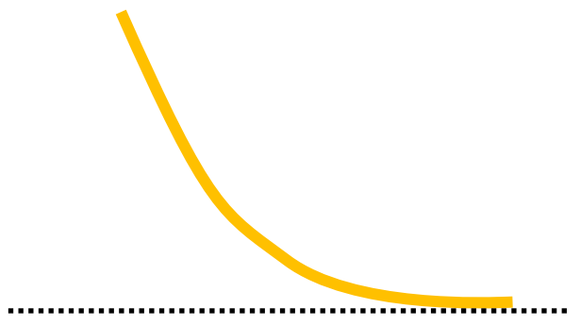
Squared loss:

- $w(\infty)$ depends on initial $w(0)$ and stepsize η
- May need to take $\eta \to 0$, $w(0) \to 0$ to get characterization in terms of gradient manifold



Exponential loss

- $\frac{w(\infty)}{\|w(\infty)\|}$ does NOT depend on initial $w(0)$ and stepsize η
- What happens at the beginning doesn't effect the asymptotic behavior as $\|w(\infty)\| \to \infty$
- Limit direction dominated only by the updates and hence the gradient manifold



- Role of optimization in ML extends beyond reaching **some global minima**
- Implicit regularization plays a crucial role in generalization of over parameterized models
- Understanding **specific global minimum** reached by an algorithm is important!

Different optimization algorithms

⇒ different implicit bias

⇒ different generalization