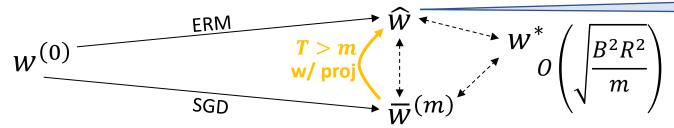
Introduction to Machine Learning TTIC 31020

Prof. Nati Srebro

Lecture 11:
 Multi-Pass SGD
 Online Learning
The Inductive Bias of Optimization





Direct SA (SGD) Approach: $\min L_S(w)$

Initialize
$$w^{(0)} = 0$$

At iteration t:

- Draw $x_t, y_t \sim \mathcal{D}$
- If $y_t \langle w^{(t)}, \phi(x_t) \rangle < 1$, $w^{(t+1)} \leftarrow w^{(t)} + \eta_t y_t \phi(x_t)$ else: $w^{(t+1)} \leftarrow w^{(t)}$

Return
$$\overline{w}^{(T)} = \frac{1}{T} \sum_{t=1}^{T} w^{(t)}$$

- Fresh sample at each iteration, m=T• one pass over the data
- No need to project nor require $||w|| \le B$
- Implicit regularization via early stopping

SGD on ERM:

$$\min_{\|w\|_2 \le B} L_S(w)$$

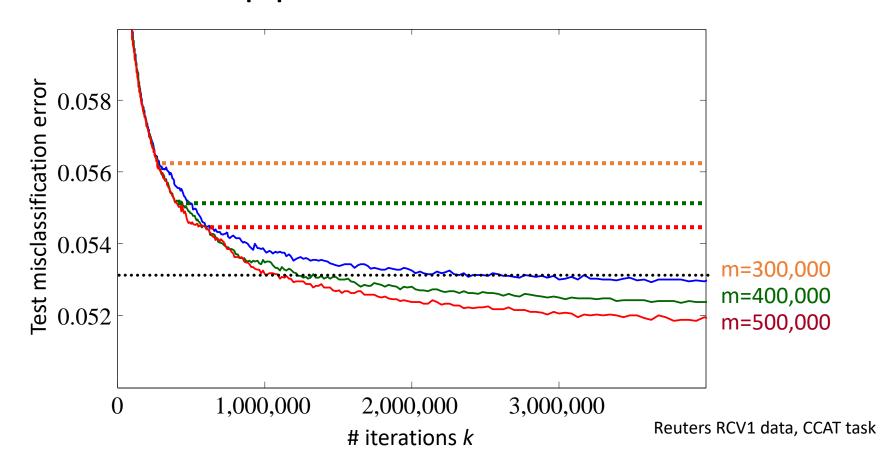
Draw
$$(x_1, y_1), \dots, (x_m, y_m) \sim \mathcal{D}$$

Initialize $w^{(0)} = 0$

At iteration t:

- Pick $i \in 1 \dots m$ at random
- If $y_i \langle w^{(t)}, \phi(x_i) \rangle < 1$, $w^{(t+1)} \leftarrow w^{(t)} + \eta_t y_i \phi(x_i)$ else: $w^{(t+1)} \leftarrow w^{(t)}$
- $w^{(t+1)} \leftarrow proj \ w^{(t+1)} \ to \ ||w|| \le B$ Return $\overline{w}^{(T)} = \frac{1}{T} \sum_{t=1}^{T} w^{(t)}$
- Can have T > m iterations (multiple passes)
- Need to project to $||w|| \le B$
- Explicit regularization via ||w||

Mixed Approach: SGD on ERM



- The mixed approach (reusing examples) can make sense
- Still: fresh samples are better
 With a larger training set, can reduce generalization error faster
 Larger training set means less runtime to get target generalization error

Direct SA/SGD Approach

(Learning as Stochastic Optimization)

SGD on the objective $L_{\mathcal{D}}(w)$

SGD is the Learning Rule

One pass/"online", T = m (processes each example once, one "epoch" over the data)

SGD on ERM

(Learning *using* Stochastic Optimization)

SGD on $L_{S}(w)$

Learning rule: ERM(S) = \widehat{w}_B = arg $\min_{\|w\|_2} L_S(w)$

or $RERM(S) = \widehat{w}_{\lambda} = \arg\min L_S(w) + \lambda ||w||_2^2$

SGD as an Optimization Algorithm for min

Multiple passes/epochs, can have T > m (can processes examples multiple times)

Online learning:

At each iteration t = 1, 2, ...

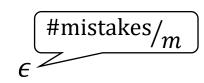
- Receive instance x_t
- Predict a label $\hat{y}_t = h^{(t)}(x_t)$
- Receive label y_t ,
- Update $h^{(t+1)}$ based on (x_t, y_t)

Stochastic Approximation (e.g. SGD):

At each iteration t = 1, 2, ...receive (x_t, y_t)

update $h^{(t+1)}$ based on (x_t, y_t)

• Goal in realizable case $(\exists_{h^* \in \mathcal{H}} h^*(x_t) = y_t)$: #mistakes (ie $h^{(t)}(x_t) \neq v_t$) $\frac{1}{m} \sum_t \ell^{01} (h^{(t)}(x_t), y_t) \leq$



• Goal in agnostic case: regret versus best $h^* \in \mathcal{H}$ in hindsight

regret versus best
$$h^* \in \mathcal{H}$$
 in hindsight
$$\frac{1}{m} \sum_{t} \ell(h^{(t)}(x_t), y_t) \leq \inf_{h^* \in \mathcal{H}} \frac{1}{m} \sum_{t} \ell(h^*(x_t), y_t) + \epsilon$$
 regret

Online regret guarantees beyond scope of course

Online Gradient Descent

Online learning:

At each iteration t = 1, 2, ...

- Receive instance x_t
- Predict a label $\hat{y}_t = h_{w^{(t)}}(x_t)$
- Receive label y_t , suffer loss $\ell(h_{w^{(t)}}, y_t)$
- Update $w^{(t+1)}$ based on (x_t, y_t)

$$w^{(t+1)} \leftarrow w^{(t)} - \eta_t \nabla_w \ell(h_{w^{(t)}}(x_t), y_t)$$

$$= w^{(t)} - \eta_t \nabla_w \ell(\langle w^{(t)}, \phi(x_t) \rangle, y_t)$$

$$= w^{(t)} - \eta_t \ell'(\langle w^{(t)}, \phi(x_t) \rangle, y_t) \phi(x_t)$$

• If $\ell(h_w(x), y)$ is convex and ρ -Lipschitz in w

$$\frac{1}{m} \sum_{t} \ell(h_{w^{(t)}}, y_{t}) \leq \inf_{\|w\|_{2} \leq B} \frac{1}{m} \sum_{t} \ell(h_{w}(x_{t}), y_{t}) + \sqrt{\frac{B^{2} \rho^{2}}{m}}$$

For linear pred

 $h_w(x) = \langle w, \phi(x) \rangle$

• If $h_w(x) = \langle w, \phi(x) \rangle$, $\|\phi(x)\|_2 \le R$ and $\ell(z, y)$ is 1-Lipschitz in z:

$$\frac{1}{m} \sum_{t} \ell(\langle w^{(t)}, \phi(x_t) \rangle, y_t) \le \inf_{\|w\|_2 \le B} \frac{1}{m} \sum_{t} \ell(\langle w, \phi(x_t) \rangle, y_t) + \sqrt{\frac{B^2 R^2}{m}}$$

Online regret guarantees beyond scope of course

Perceptron as OGD

Online learning:

At each iteration t = 1, 2, ...

- Receive instance x_t
- Predict a label $\hat{y}_t = h_{w^{(t)}}(x_t)$
- Receive label y_t , suffer loss $\ell(h_{w^{(t)}}, y_t)$
- Update $w^{(t+1)}$ based on (x_t, y_t)

$$w^{(t+1)} \leftarrow w^{(t)} - \eta_t \nabla_w \ell(h_{w^{(t)}}(x_t), y_t)$$

$$= w^{(t)} - \eta_t \nabla_w \ell(\langle w^{(t)}, \phi(x_t) \rangle, y_t)$$

$$= w^{(t)} - \eta_t \ell'(\langle w^{(t)}, \phi(x_t) \rangle, y_t) \phi(x_t)$$

At iteration t:

- Receive x_t
- Predict $\hat{y}_t = sign(\langle w^{(t)}, \phi(x_t) \rangle)$
- Receive y_t
- If $y_t \neq \hat{y}_t$, $w^{(t+1)} \leftarrow w^{(t)} + y_t \phi(x_t)$ else: $w^{(t+1)} \leftarrow w^{(t)}$



Frank Rosenblatt

$$\ell'(\langle w^{(t)}, \phi(x_t) \rangle, y_t) = \begin{cases} -1, & y_t \neq \hat{y}_t = sign(\langle w^{(t)}, \phi(x_t) \rangle \\ 0, & y_t = sign(\langle w^{(t)}, \phi(x_t) \rangle \end{cases}$$

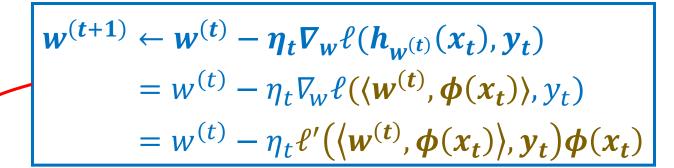
Perceptron as OGD

 $\ell(z,y) = [-zy]_{+}$

Online learning:

At each iteration t = 1, 2, ...

- Receive instance x_t
- Predict a label $\hat{y}_t = h_{w^{(t)}}(x_t)$
- Receive label y_t , suffer loss $\ell(h_{w^{(t)}}, y_t)$
- Update $w^{(t+1)}$ based on (x_t, y_t)



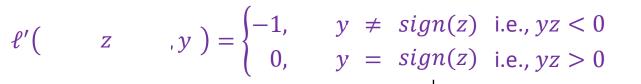
At iteration t:

- Receive x_t
- Predict $\hat{y}_t = sign(\langle w^{(t)}, \phi(x_t) \rangle)$
- Receive y_t
- If $y_t \neq \widehat{y}_t$, $w^{(t+1)} \leftarrow w^{(t)} + y_t \phi(x_t)$ else: $w^{(t+1)} \leftarrow w^{(t)}$



A STATE OF THE STA

Frank Rosenblatt



$$\frac{1}{m} \sum_{t} \ell(h_{w^{(t)}}, y_t) \le \inf_{w} \frac{1}{m} \sum_{t} \ell(h_{w}(x_t), y_t) + Regret$$

Online algorithm A

e.g. Online Gradient Descent:

$$w^{(t+1)} \leftarrow w^{(t)} \\ -\eta \nabla_w \left(h_{w^{(t)}}(x_t, y_t) \right)$$

or online Perceptron

Realizable Online-to-Batch

$$(if \exists w^* L_S(w^*) = 0)$$

Input:
$$S = (x_1, y_1) ... (x_m, y_m) \sim \mathcal{D}^m$$

While $y_i w^{(t)}(x_i) < 0$, feed (x_i, y_i) into A to get $w^{(t+1)}$

Output $w^{(T)}$

Empirical Optimization: $L_S(w^{(T)}) = 0$

Generalization:
$$\mathbb{E}[L_{\mathcal{D}}(w^{(T)})] \leq \frac{\text{\#mistakes}}{m} = Regret$$

One-Pass Online-to-Batch

Input:
$$S = (x_1, y_1) ... (x_m, y_m) \sim \mathcal{D}^m$$

For
$$t = 1 ... m$$
,

feed (x_t, y_t) into \underline{A} to get $w^{(t+1)}$

Output
$$\overline{w} = \frac{1}{m} \sum w^{(t)}$$

Generalization:

$$\mathbb{E}[L_{\mathcal{D}}(\overline{w})] \leq \inf_{w^*} L_{\mathcal{D}}(w^*) + Regret$$

Onlined Gradient Descent

[Zinkevich 03]

online2stochastic
[Cesa-Binachi et al 04]

Stochastic Gradient Descent [Nemirovski Yudin 78]

Online Learning vs Stochastic Approximation

- In both Online Setting and Stochastic Approximation
 - Receive samples sequentially
 - Update predictor after each sample

• But, in Online Setting:

- Objective is empirical regret, i.e. behavior on observed instances
- Every point is both a training point and a test point
- (x_t, y_t) chosen arbitrarily (no distribution involved), could be non stationary, non independent, adapt based on predictor, anything goes
- Whereas in Stochastic Approximation:
 - Objective is $L(h) = \mathbb{E}_{x,y}[loss(h(x),y)]$, i.e. behavior on "future" samples $(x,y) \sim \mathcal{D}$
 - i.i.d. *training* samples $(x_t, y_t) \sim \mathcal{D}$
 - Have same source distribution \mathcal{D} for train and test crucial
- Stochastic Approximation is a computational approach, Online Learning is an analysis setup
 - E.g. "Majority" is a valid online algorithm and makes sense to analyze as such

Direct SA/SGD Approach

(Learning *as* Stochastic Optimization)

SGD on the objective $L_{\mathcal{D}}(w)$

SGD as a Learning Rule

One pass/epoch: "online", T = m (processes each example once)

Generalization from SGD regret guarantee

$$L_{\mathcal{D}}(\overline{w}^T) \le L_{\mathcal{D}}(w^*) + O\left(\sqrt{\frac{\|w^*\|_2^2 \|\phi\|_2^2}{T}}\right)$$

What is the inductive bias?

How and where is it specified or used in SGD?

SGD on ERM

(Learning *using* Stochastic Optimization)

SGD on $L_{\mathbf{S}}(w)$

Learning rule: ERM(S) = \widehat{w}_B = arg min $L_S(w)$

or $RERM(S) = \widehat{w}_{\lambda} = \arg\min L_S(w) + \lambda ||w||_2^2$

SGD as an Optimization Algorithm for min

Multiple passes/epochs, can have T > m (can processes examples multiple times)

Explicit complexity control: $||w||_2 \le B \text{ or } +\lambda ||w||_2^2$

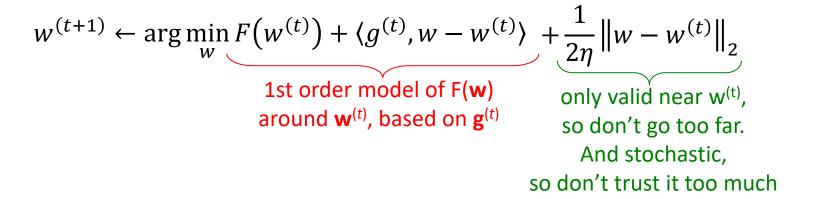
Generalization from explicit complexity control:

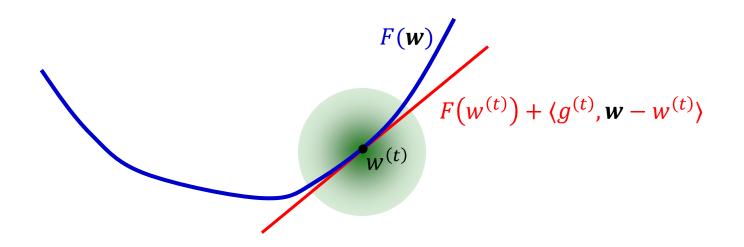
$$L_{\mathcal{D}}(\widehat{w}_B) \le L_{\mathcal{D}}(w^*) + O\left(\sqrt{\frac{\|w^*\|_2^2 \|\phi\|_2^2}{m}}\right)$$

Explicit inductive bias: $||w||_2$

Where's the Regularization

• Gradient Descent seems to be regularizing with $||w||_2$. How?





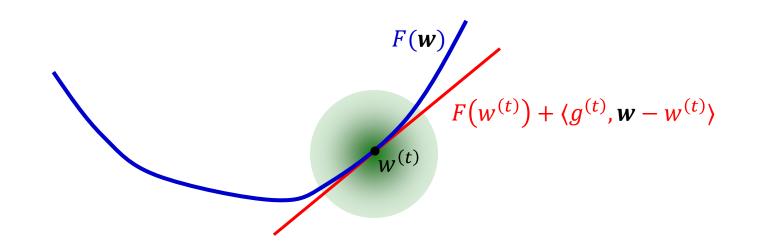
Where's the Regularization

• Gradient Descent seems to be regularizing with $||w||_2$. How?

$$w^{(t+1)} \leftarrow \arg\min_{w} F(w^{(t)}) + \langle g^{(t)}, w - w^{(t)} \rangle + \frac{1}{2\eta} \|w - w^{(t)}\|_{2}$$

$$= \arg\min_{w} \langle g^{(t)}, w \rangle + \frac{1}{2\eta} \|w - w^{(t)}\|_{2}$$

$$= w^{(t)} - \eta g^{(t)}$$



- SGD (at least on convex problems) implicitly regularizes using $||w||_2$
 - #iterations $T \approx \text{sample complexity } m \propto ||w||_2^2$
 - Generalization/suboptimality controlled in terms of $||w||_2 \rightarrow$ this is the inductive bias
 - Alternative to $||w||_2 \le B$ or adding $\lambda ||w||_2$ for injecting $||w||_2$ inductive bias (same guarantee)
- What about other regularizers R(w) / inductive biases??
 - Can apply SGD to regularized or constrained ERM:

$$\min_{R(w) \le B} L_S(w)$$
 or $\min L_S(w) + \lambda R(w)$

Sample complexity m controlled by $R(w^*)$,

...but #iterations T controlled by $||w^*||_2$

Other optimization methods related to other regularizers / inductive biases

(generic answer for convex R(w) and convex (ie linear) learning problems: Stochastic Mirror Descent with potential function corresponding to R(w)—beyond scope of this course)

- Stochastic Gradient Descent as a Learning Algorithm:
 - One pass over the data!
- What if we do multiple passes over the data?
- Or what about batch gradient descent?

Can Batch Gradient Descent also help generalization (inject inductive bias)?

$$\begin{split} \min_{w} L_S(w) & \text{using } w^{(t+1)} \leftarrow w^{(t)} - \eta_t \nabla L_S(w^{(t)}) \\ w^{(t)} & \xrightarrow{t \to \infty} \arg\min L_S(w) \quad \text{, but which minimizer??} \end{split}$$

- Consider $h_w(x) = \langle w, \phi(x) \rangle$, $\phi(x) \in \mathbb{R}^D$, $D \gg m$, $\ell(h_w(x), y) = |h_w(x) y|$
- If data in ``general position'': $\exists w L_S(w) = 0$, in fact an entire D m dim space of minimizers!

Claim: starting from $w^{(0)} = 0$, $w^{(t)} \xrightarrow{t \to \infty} \arg \min ||w||_2$ s.t. $L_S(w) = 0$ Proof:

$$(1) \ w^{(t)} \in span(\phi(x_1), ..., \phi(x_m))$$

$$\nabla L_S(w) = \sum \ell'(...) \phi(x_i) \in span(\phi(x_1), ..., \phi(x_m))$$

$$w^{(t)} = -\sum \eta_t \nabla L_S(w^{(j)}) \in span(\nabla L_S(w^{(j)})) \subseteq span(\phi(x_1), ..., \phi(x_m))$$

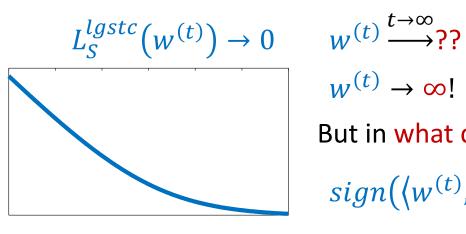
(2) If $w \in span(\phi(x_1), ..., \phi(x_m))$ and $\langle w, \phi(x_i) \rangle = y_i$, then it's the min norm solution consider $w + w_{\parallel} + w_{\perp}$. Any $w_{\perp} \neq 0$ would violate constraints, and any $w_{\parallel} \neq 0$ would increase norm

Can Batch Gradient Descent also help generalization (inject inductive bias)?

$$\min_{w} L_{S}(w) \qquad \text{using } w^{(t+1)} \leftarrow w^{(t)} - \eta_{t} \nabla L_{S}^{lgstc}(w^{(t)})$$

$$w^{(t)} \xrightarrow{t \to \infty} \arg\min L_{S}(w) \quad \text{, but which minimizer??}$$

- Consider $h_w(x) = \langle w, \phi(x) \rangle$, $\phi(x) \in \mathbb{R}^D$, $D \gg m$, $\ell^{lgstc}(h_w(x), y) = \log(1 + e^{-yh_w(x)})$
- Data linear separable: $\exists w \ \forall_i y_i \langle w, \phi(x_i) \rangle > 0$

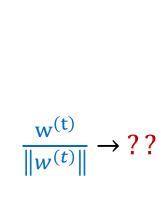


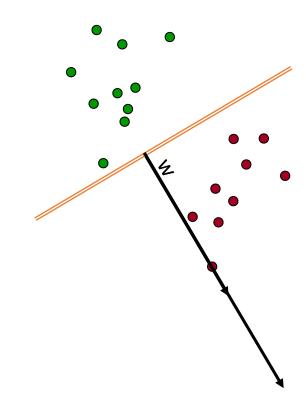
$$w^{(t)} \xrightarrow{t \to \infty}$$
??

$$w^{(t)} \rightarrow \infty!$$

But in what direction?

$$sign(\langle w^{(t)}, \phi(x) \rangle) \rightarrow ??$$
 $\frac{w^{(t)}}{\|w^{(t)}\|} \rightarrow ??$





Can Batch Gradient Descent also help generalization (inject inductive bias)?

$$\min_{w} L_{S}(w) \qquad \text{using } w^{(t+1)} \leftarrow w^{(t)} - \eta_{t} \nabla L_{S}^{lgstc}(w^{(t)})$$

$$w^{(t)} \xrightarrow{t \to \infty} \arg\min L_{S}(w) \qquad \text{, but which minimizer??}$$

- Consider $h_w(x) = \langle w, \phi(x) \rangle$, $\phi(x) \in \mathbb{R}^D$, $D \gg m$, $\ell^{lgstc}(h_w(x), y) = \log(1 + e^{-yh_w(x)})$
- Data linear separable: $\exists w \ \forall_i y_i \langle w, \phi(x_i) \rangle > 0$

$$L_S^{lgstc}(w^{(t)}) \to 0 \qquad w^{(t)} \xrightarrow{t \to \infty} ??$$

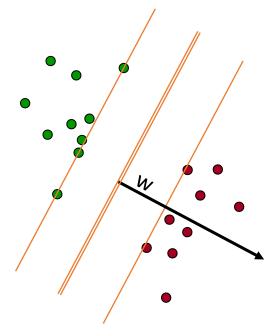
$$w^{(t)} \xrightarrow{t \to \infty} ??$$

$$w^{(t)} \rightarrow \infty!$$

But in what direction?

$$sign(\langle w^{(t)}, \phi(x) \rangle) \rightarrow ??$$
 $\frac{w^{(t)}}{\|w^{(t)}\|} \rightarrow ??$

$$\frac{\mathbf{w}^{(t)}}{\|\mathbf{w}^{(t)}\|} \rightarrow ??$$



Claim:
$$\frac{w(t)}{\|w(t)\|_2} \xrightarrow{t \to \infty} \frac{\widehat{w}}{\|\widehat{w}\|_2}$$

$$\widehat{w} = \arg\min \|w\|_2 \ s.t. \ \forall_i y_i \langle w, x_i \rangle \ge 1$$

• Gradient Descent (or Multi-Pass SGD) on $L_S(w)$ converges to $\arg\min \|w\|_2 s$. t. $L_S(w) = 0$

or
$$\propto \arg\min \|w\|_2 \ s. \ t. \ L_s^{\text{margin}}(w) = 0 \ (\text{with } \ell^{lgstc})$$

$$\equiv \text{MDL for } \|w\|_2$$

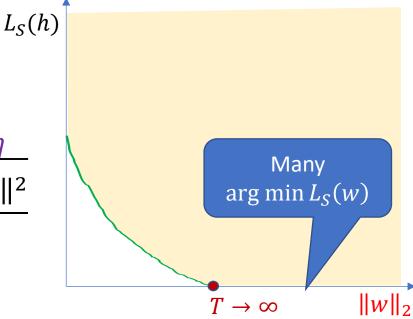
(with
$$\ell^{abs}(h_w(x), y) = |h_w(x) - y|$$
 or $\ell^{sq}(h_w(x), y) = (h_w(x) - y)^2$)

One-Pass ("Online") Stochastic Gradient Descent

Learning with $\|w\|_2$ inductive bias

complexity/fit tradeoff controlled by stepsize ("learning rate") η

$$L(w) \le \inf_{\|\mathbf{w}^*\|_2 \le \eta \|\phi\|_m} L(w^*) + \eta \|\phi\|^2 \le \inf_{\|\mathbf{w}^*\|_2 \le B} L(w^*) + \sqrt{\frac{B^2 \|\phi\|^2}{m}}$$
with $n = \frac{B}{\|\mathbf{w}^*\|_2}$



• Gradient Descent (or Multi-Pass SGD) on $L_S(w)$ converges to $\arg\min \|w\|_2 s$. t. $L_S(w) = 0$

or
$$\propto \arg\min \|w\|_2 \ s. \ t. \ L_s^{\text{margin}}(w) = 0 \ (\text{with } \ell^{lgstc})$$

$$\equiv \text{MDL for } \|w\|_2$$

(with
$$\ell^{abs}(h_w(x), y) = |h_w(x) - y|$$
 or $\ell^{sq}(h_w(x), y) = (h_w(x) - y)^2$)

- Gradient Descent or Multi-Pass SGD with Early Stopping provides complexity control related to $\|w\|_2$ generalization similar to RERM, $\arg\min L_S(w) + \lambda \|w\|_2$ tradeoff controlled by stepsize and stopping time (#iterations)
- One-Pass ("Online") Stochastic Gradient Descent

Learning with $||w||_2$ inductive bias

complexity/fit tradeoff controlled by stepsize ("learning rate") η

$$L(w) \le \inf_{\|\mathbf{w}^*\|_2 \le \eta \|\phi\|_m} L(w^*) + \eta \|\phi\|^2 \le \inf_{\|\mathbf{w}^*\|_2 \le B} L(w^*) + \sqrt{\frac{B^2 \|\phi\|^2}{m}}$$
with $\eta = \frac{B}{\|\phi\|\sqrt{m}}$

Draw $(x_1, y_1), ..., (x_m, y_m) \sim \mathcal{D}$

Initialize $w^{(0)} = 0$

At iteration t=1...T:

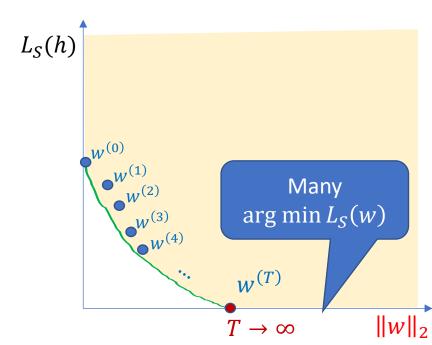
- Pick $i \in 1 \dots m$ at random
- If $y_i \langle w^{(t)}, \phi(x_i) \rangle < 1$, $w^{(t+1)} \leftarrow w^{(t)} + \eta_t y_i \phi(x_i)$ else: $w^{(t+1)} \leftarrow w^{(t)}$
- $w^{(t+1)} \leftarrow proj \ w^{(t+1)} \ to \ ||w|| \le B$ Return $\overline{w}^{(T)} = \frac{1}{T} \sum_{t=1}^{T} w^{(t)}$

• Gradient Descent (or Multi-Pass SGD) on $L_S(w)$ converges to $\arg\min \|w\|_2 s$. t. $L_S(w) = 0$

```
or \propto \arg\min \|w\|_2 \ s.\ t.\ L_s^{\mathrm{margin}}(w) = 0 \ (\text{with } \ell^{lgstc})
\equiv \mathrm{MDL} \ \mathrm{for} \ \|w\|_2
```

(with $\ell^{abs}(h_w(x), y) = |h_w(x) - y|$ or $\ell^{sq}(h_w(x), y) = (h_w(x) - y)^2$)

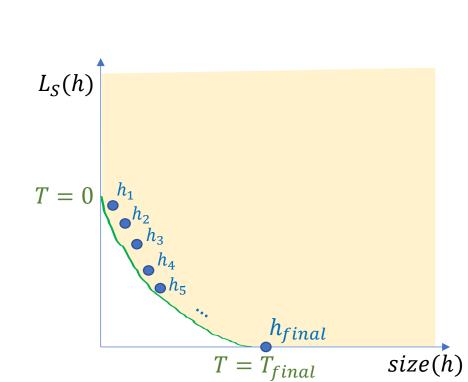
• Gradient Descent or Multi-Pass SGD with Early Stopping provides complexity control related to $\|w\|_2$ generalization similar to RERM, $\arg\min L_S(w) + \lambda \|w\|_2$ tradeoff controlled by stepsize and stopping time (#iterations)

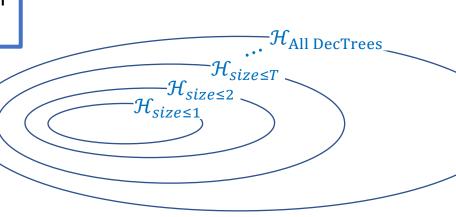


Greedy Decision Tree Construction, minimizing $L_S(h)$ Init empty decision tree h_0 While some nodes in h_t are impure (have ≥ 1 train label): Pick node v and feature that maxs train error reduction Split v according to predicate to obtain h_{t+1}

$$h_{final} \approx \arg\min_{L_S(h)=0} size(h_T)$$

- But early stopping after T iterations: $size(h_T) \leq T$
- Early stopping corresponds to controlling the inductive bias "decision tree size"
- How early we step
 ≡ balance between fit and complexity
 ≡ where we are on regularization path





- One-Pass ("Online") Stochastic Gradient Descent Learning with $\|w\|_2$ inductive bias complexity/fit tradeoff controlled by stepsize ("learning rate") η
- Multi-Pass SGD or Batch Gradient Descent with Early Stopping provides complexity control related to $\|w\|_2$ generalization properties similar to RERM, $\arg\min L_S(w) + \lambda \|w\|_2$ tradeoff controlled by stepsize and stopping time (#iterations)
- Multi-Pass SGD or Batch Gradient Descent to Convergence \approx MDL, $\arg\min \|w\|_2$

- When $D \gg m$, for $h_w(x) = \langle w, \phi(x) \rangle$, there are MANY $\arg \min L_s(w)$
- Gradient Descent on $L_S(w)$ converges to $\underset{\text{arg min}}{\text{arg min}} \|w\|_2 s.t. L_s(w) = 0$ (with $\ell^{abs}(h_w(x), y) = |h_w(x) y|$ or or $\propto \underset{\text{arg min}}{\text{arg min}} \|w\|_2 s.t. L_s^{\text{margin}}(w) = 0$ (with ℓ^{lgstc}) $\ell^{sq}(h_w(x), y) = (h_w(x) y)^2$)

$$\equiv$$
 MDL for $||w||_2$

• This is specific to the optimization method!

Instead:

Coordinate descent:

$$i^{(t)} = \arg \max |\partial_i L_S(w^{(t)})|$$

$$w^{(t+1)} = \arg \min L(w) \quad w = w^{(t)} + \eta e_i$$

Bias towards sparser solutions!

With logistic loss, $\rightarrow \propto \arg \min ||w||_1 s. t. L_s^{\text{margin}}(w) = 0$

