Inductive Bias, Generalization and the role of Optimization in Deep Learning

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• **Supervised Learning:** find \( h: \mathcal{X} \rightarrow \mathcal{Y} \) with small generalization error
\[
L(h) = \mathbb{E}_{(x,y) \sim \mathcal{D}} \left[ \text{loss}(h(x); y) \right]
\]
based on samples \( S \) (hopefully \( S \sim \mathcal{D}^m \)) using learning rule:
\[
A: S \mapsto h \quad \text{(i.e. } A: (\mathcal{X} \times \mathcal{Y})^* \rightarrow \mathcal{Y}^\mathcal{X} \text{)}
\]

• **No Free Lunch:** For any learning rule, there exists a source \( \mathcal{D} \) (i.e. reality), for which the learning rule yields expected error \( \frac{1}{2} \)

• More formally for any \( A, m \) there exists \( \mathcal{D} \) s.t.
\[
\mathbb{E}_{S \sim \mathcal{D}^m} \left[ L(A(S)) \right] \geq \frac{1}{2} - \frac{m}{2|\mathcal{X}|}
\]

• **Inductive Bias:**
  • Some realities (sources \( \mathcal{D} \)) are less likely; design \( A \) to work well on more likely realities
    e.g., by preferring certain \( y|x \) (i.e. \( h(x) \)) over others
  • Assumption or property of reality \( \mathcal{D} \) under which \( A \) ensures good generalization error
    e.g., \( \exists h \in \mathcal{H} \text{ with low } L(h) \)
    e.g., \( \exists h \) with low “complexity” \( c(h) \) and low \( L(h) \)
Flat Inductive Bias

- "Flat" inductive bias: \( \exists h^* \in \mathcal{H} \) with low \( L(h^*) \)
- (Almost) optimal learning rule:
  \[
  \text{ERM}_{\mathcal{H}}(S) = \hat{h} = \arg\min_{h \in \mathcal{H}} L_S(h)
  \]
- Guarantee (in expectation over \( S \sim \mathcal{D}^m \)):
  \[
  L(\text{ERM}_{\mathcal{H}}(S)) \leq L(h^*) + \mathcal{R}_m(\mathcal{H}) \approx L(h^*) + \sqrt{\frac{O(\text{capacity}(\mathcal{H}))}{m}}
  \]
  \( \Rightarrow \) can learn with \( O(\text{capacity}(\mathcal{H})) \)
- E.g.
  - For binary classification, \( \text{capacity}(\mathcal{H}) = VCDim(\mathcal{H}) \)
  - Vapnik-Chervonenkis (VC) dimension: largest number of points \( D \) that can be labeled (by some \( h \in \mathcal{H} \)) in every possible way (i.e. for which the inductive bias is uninformative)
  - For linear classifiers over \( d \) features, \( VCDim(\mathcal{H}) = d \)
  - Usually with \( d \) parameters, \( VCDim(\mathcal{H}) \approx \tilde{O}(#\text{params}) \)
  - Always: \( VCDim(\mathcal{H}) \leq \log |\mathcal{H}| = \#\text{bits} \)
Flat Inductive Bias

• “Flat” inductive bias: $\exists h^* \in \mathcal{H}$ with low $L(h^*)$

• (Almost) optimal learning rule:

$$\text{ERM}_{\mathcal{H}}(S) = \hat{h} = \arg\min_{h \in \mathcal{H}} L_S(h)$$

• Guarantee (in expectation over $S \sim \mathcal{D}^m$):

$$L(\text{ERM}_{\mathcal{H}}(S)) \leq L(h^*) + \mathcal{R}_m(\mathcal{H}) \approx L(h^*) + \sqrt{\frac{O(\text{capacity}(\mathcal{H}))}{m}}$$

$\Rightarrow$ can learn with $O(\text{capacity}(\mathcal{H}))$

• E.g.

• For binary prediction, $\text{capacity}(\mathcal{H}) = \text{VCdim}(\mathcal{H})$
• For linear predictors over $d$ features, $\text{capacity}(\mathcal{H}) = d$
• Usually with $d$ parameters, $\text{capacity}(\mathcal{H}) \approx O(\#\text{params})$
• Always: $\text{capacity}(\mathcal{H}) \leq \#\text{bits}$
• For linear predictors with $\|w\|_2 \leq B$, with logistic loss and normalized data: $\text{capacity}(\mathcal{H}) = B^2$
• We want model classes (hypothesis classes) that:
  • Are expressive enough to capture reality well
  • Have small enough capacity to allow generalization
Complexity Measure as Inductive Bias

- **Complexity measure**: mapping $c: \mathcal{Y}^\mathcal{X} \to [0, \infty]$ 
- Associated inductive bias: $\exists h$ with small $c(h)$ and small $L(h)$ 
- Learning rule: $SRM_{\mathcal{H}}(S) = \arg\min L(h), c(h)$ 
  e.g. $\arg\min L(h) + \lambda c(h)$ or $\arg\min L(h)$ s.t. $c(h) \leq B$ and choose $\lambda$ or $B$ using cross-validation 
- Guarantee: 
  $$L(SRM_{\mathcal{H}}(S)) \leq \approx L(h^*) + \sqrt{\frac{\text{capacity}(\mathcal{H}_{c(h^*)})}{m}}$$ 
- E.g.: 
  - Degree of poly 
  - Sparsity 
  - $\|w\|$
reality
Beyond ERM: Implicit Inductive Bias

- The one-pass-SGD learning rule for linear predictors $h_w(x) = \langle w, x \rangle$
  $$SGD(S) = \frac{1}{m} \sum_{i=1}^{m} w_i \text{ where } w_{i+1} = w_i - \eta \nabla \text{loss}(\langle w, x_i \rangle; y_i)$$

- Theorem: If $|\text{loss}'| \leq 1$ and $\|x\| \leq 1$, then with $w_0 = 0$ and appropriate $\eta$
  $$L(SGD(S)) \leq L(w^*) + \sqrt{\frac{\|w\|_2^2}{m}}$$

- Inductive bias: $c(h_w) = \|w\|_2$
Explicit and Implicit Inductive Bias

\[ \mathcal{H} \text{ or } c(h) \]

\[ \|w\|_2 \]

\[ P(y|x) \text{ smooth w.r.t } d(x, x') \]

sparsity or \[ \|w\|_1 \]

\[ c(h) \]

ERM or SRM

SGD

Nearest Neighbor

Exp GD (Mult Weights)

Mirror Descent with potential \( \approx c(h) \)
Feed-Forward Neural Networks
(The Multilayer Perceptron)

Architecture:
• Directed Acyclic Graph $G(V,E)$. Units (neurons) indexed by vertices in $V$.
  • “Input Units” $v_1 \ldots v_d \in V$, with no incoming edges and $o[v_i] = x[i]$
  • “Output Unit” $v_{out} \in V$, $h_w(x) = o[v_{out}]$
• “Activation Function” $\sigma : \mathbb{R} \to \mathbb{R}$. E.g. $\sigma(z) = \text{sign}(z)$ or $\sigma(z) =$

Parameters:
• Weight $w[u \to v]$ for each edge $u \to v \in E$
Feed-Forward Neural Networks as a Hypothesis Class

$$\mathcal{H}_{G(V,E),\sigma} = \{ h_{G(V,E),\sigma,w} \mid w: E \rightarrow \mathbb{R} \}$$

or $$\mathcal{H}_{G(V,E),\sigma}^{sign} = \{ sign(h_{G(V,E),\sigma,w}) \mid w: E \rightarrow \mathbb{R} \}$$

• Hypothesis class specified by: (ie we decide on this in advance)
  • Graph $G(V,E)$
    • $V$ includes input, output and “hidden” nodes
  • Activation function $\sigma$
    e.g. $\text{sign}(z)$,
    $\text{tanh}(z)$, $\text{sigmoid}(z) = \frac{1}{1+e^{-z}}$,
    $\text{relu}(z) = \max(0,z)$,
    $\text{ramp}(z) = \text{clip}_{[-1,1]}(z)$

• Hypothesis specified by: (ie we need to learn)
  • Weights $w$, with weight $w[u \rightarrow v]$ for each edge $u \rightarrow v \in E$
Feed Forward Neural Networks

• Fix architecture (connection graph $G(V, E)$, transfer $\sigma$)

$$\mathcal{H}_{G(V,E),\sigma} = \{ f_w(x) = \text{output of net with weights } w \}$$

• Capacity / Generalization ability / Sample Complexity

• Expressive Power / Approximation
Capacity (Sample Complexity) of NN

- \#params = \(|E|\) (number of weights we need to learn)
- More formally: \(VCdim(H_{G(V,E),sig}) = O(|E| \log |E|)\)
- Other activation functions?
  - \(VCdim(H_{G(V,E),\sin}) = \infty\) even with single unit and single real-valued input
  - For \(\sigma(z) = \text{sigmoid}(z) = \frac{1}{1+e^{-z}}\):
    \[\Omega(|E|^2) \leq VCdim(H_{G(V,E),\text{sigmoid}}) \leq O(|E|^4)\]
  - For piecewise linear, e.g. \(ramp(z) = \text{clip}_{[-1,1]}(z)\) or \(ReLU(z) = \max(0, z)\):
    \[\Omega \left( |E|L \log \frac{|E|}{L} \right) \leq VCdim(H_{G,\sigma}) \leq O(|E|L \log |E|)\]
- With integer weights \(\in [-B, \ldots, B]\):
  \[VCdim(H_{G(V,E),\sigma}) \leq \log |H_{G(V,E),\sigma}| \leq 2|E| \log B\]
Feed Forward Neural Networks

- Fix architecture (connection graph $G(V, E)$, transfer $\sigma$)

$$\mathcal{H}_{G(V, E), \sigma} = \{ f_w(x) = \text{output of net with weights } w \}$$

- Capacity / Generalization ability / Sample Complexity
  - $\tilde{O}(|E|)$ (number of edges, i.e. number of weights)
  (with threshold $\sigma$, or with RELU and finite precision; RELU with inf precision: $\tilde{O}(|E| \cdot \text{depth})$)

- Expressive Power / Approximation
What can Feed-Forward Networks Represent?

• Any function over $\mathcal{X} = \{\pm 1\}^n$
  • With a single hidden layer, using DNF (hidden layer does AND, output does OR)
  • $|V| = 2^n$, $|E| = n2^n$
  • Like representing the truth table directly...

• Universal Representation Theorem: Any continuous functions $f : [0,1]^n \to \mathbb{R}$ can be approximated to within any $\epsilon$ by a feed-forward network with sigmoidal (or almost any other) activation and a single hidden layer.
  • Size of layer exponential in $n$
What can SMALL Networks Represent?

• Intersection of halfspaces
  • Using single hidden layer

• Union of intersection of halfspaces (and also sorting, more fun stuff, ...)
  • Using two hidden layers
What can SMALL Networks Represent?

• Intersection of halfspaces
  • Using single hidden layer

• Union of intersection of halfspaces (and also sorting, more fun stuff, ...)
  • Using two hidden layers

• Functions representable by a small logical circuit
  • Implement AND using single unit, negation by reversing weight

• Functions that depend on lower level features
Multi-Layer Feature Learning
Feed Forward Neural Networks

• Fix architecture (connection graph $G(V, E)$, transfer $\sigma$)

$$\mathcal{H}_{G(V,E),\sigma} = \{ f_w(x) = \text{output of net with weights } w \}$$

• Capacity / Generalization ability / Sample Complexity
  
  • $\tilde{O}(|E|)$ (number of edges, i.e. number of weights)
    (with threshold $\sigma$, or with RELU and finite precision; RELU with inf precision: $\tilde{\Theta}(|E| \cdot \text{depth})$)

• Expressive Power / Approximation
  
  • Any continuous function with huge network
  • Lots of interesting things naturally with small networks
  • Any time $T$ computable function with network of size $\tilde{O}(T)$
Free Lunches

- **ML as an Engineering Paradigm**: Use data and examples, instead of expert knowledge and tedious programming, to automatically create efficient systems that perform complex tasks

- We only care about \( \{h|h \text{ is an efficient system}\} \)

- **Free Lunch**: \( TIME_T = \{h|h \text{ comp. in time } T\} \) has capacity \( O(T) \) and hence learnable with \( O(T) \) samples, e.g. using ERM

- Even better: \( PROG_T = \{\text{program of length } T\} \) has capacity \( O(T) \)
  - \( |PROG_T| = 128^T \) \( \Rightarrow \) capacity \( \leq \log|PROG_T| = O(T) \)

- Problem: ERM for above is not computable!

- Modified ERM for \( TIME_T \) (truncating exec. time) is NP-complete

- \( P=NP \) \( \Rightarrow \) Universal Learning is possible! (Free Lunch)

- Crypto is possible (one-way functions exist)
  \( \Rightarrow \) No poly-time learning algorithm for \( TIME_T \)
  (that is: no poly-time \( A \) and uses \( poly(T) \) samples s.t. if \( \exists h^* \in TIME_T \) with \( L(h^*) = 0 \) then \( \mathbb{E}[L(A(S))] \leq 0.499 \)
No Free (Computational) Lunch

• **Statistical No-Free Lunch**: For any learning rule $A$, there exists a source $D$ (i.e. reality), s.t. $\exists h^*$ with $L(h^*) = 0$ but $\mathbb{E}[L(A(S))] \approx \frac{1}{2}$.

• **Cheating Free Lunch**: There exists $A$, s.t. for any reality $D$ and any **efficiently computable** $h^*$, $A$ learns a predictor almost as good as $h^*$ (with $\#\text{samples}=\mathcal{O}(\text{runtime of } h^*)$).

• **Computational No-Free Lunch**: For every **computationally efficient** learning **algorithm** $A$, there is a reality $D$ s.t. there is some comp. efficient (poly-time) $h^*$ with $L(h^*) = 0$ but $\mathbb{E}[L(A(S))] \approx \frac{1}{2}$.

• **Inductive Bias**: Assumption or property of reality $D$ under which a learning **algorithm** $A$ **runs efficiently** and ensures **good generalization error**.

• $\mathcal{H}$ or $c(h)$ are **not** sufficient inductive bias if ERM/SRM not efficiently implementable, or implementation doesn’t always work (runs quickly and returns actual ERM/SRM).
Feed Forward Neural Networks

• Capacity / Generalization ability / Sample Complexity
  • $\tilde{O}(|E|)$ (number of edges, i.e. number of weights)
    (with threshold $\sigma$, or with RELU and finite precision; RELU with inf precision: $\tilde{\Theta}(|E| \cdot \text{depth})$)

• Expressive Power / Approximation
  • Any continuous function with huge network
  • Lots of interesting things naturally with small networks
  • Any time $T$ computable function with network of size $\tilde{O}(T)$

• Computation / Optimization
  • Non-convex
  • No known algorithm guaranteed to work
  • NP-hard to find weights even with 2 hidden units
  • Even if function exactly representable with single hidden layer with $\Theta(\log d)$ units, even with no noise, and even if we train a much larger network or use any other method when learning: no poly-time algorithm can ensure better-than-chance prediction
    [Kearns Valiant 94; Klivans Sherstov 06; Daniely Linial Shalev-Shwartz ‘14]
Choose your universal learner:

**Short Programs**
- Universal
- Captures anything we want with reasonable sample complexity
- Provably (worst case) hard to optimize
- Hard to optimize in practice

**Deep Networks**
- Universal
- Captures anything we want with reasonable sample complexity
-Provably (worst case) hard to optimize
- Often easy to optimize
  - Continuous
  - Amenable to local search, stochastic local search
  - Lots of empirical success
Feed Forward Neural Networks

• Capacity / Generalization ability / Sample Complexity
  • $\tilde{O}(|E|)$ (number of edges, i.e. number of weights)
    (with threshold $\sigma$, or with RELU and finite precision; RELU with inf precision: $\tilde{\Theta}(|E| \cdot \text{depth})$)

• Expressive Power / Approximation
  • Any continuous function with huge network
  • Lots of interesting things naturally with small networks
  • Any time $T$ computable function with network of size $\tilde{O}(T)$

• Computation / Optimization
  • Even if function exactly representable with single hidden layer with $\Theta(\log d)$ units, even with no noise, and even if we allow a much larger network when learning: no poly-time algorithm always works [Kearns Valiant ’94; Klivans Sherstov 06; Daniely Linial Shalev-Shwartz ’14]
  • Often easy to optimize in practice, on interesting/useful problems
  • Magic property of reality that makes local search “work”
[Neyshabur Tomioka S ICLR’15]
For valid generalization, the size of the weights is more important than the size of the network.
E.g., hard margin SVM: \( \min \|w\| \) s.t. \( L^\text{margin}_S(w) = 0 \)
for \( h_w = \langle w, \phi(x) \rangle \) with inf dim \( \phi \)
E.g., hard margin SVM: \( \min \|w\| \text{ s.t. } L_{s}^{\text{margin}}(w) = 0 \)
for \( h_w = \langle w, \phi(x) \rangle \) with inf dim \( \phi \)
AdaBoost

Test error

Training error

\[ \ell_1 \text{ margin: } \frac{\langle w, x \rangle}{\|w\|_1} \]

[Bartlett, Freund, Lee, Schapire 1998]
“Size of Weights” and Generalization

\[
\text{Norm} = \|W\|_2 = \sqrt{\sum_e w(e)^2} \quad \text{Path-Norm} = \sqrt{\sum_{\text{path}} \prod_{e \in \text{path}} w(e)^2}
\]
reality
“Size of Weights” and Generalization

Norm = $\|W\|_2 = \sqrt{\sum w(e)^2}$

Path-Norm = $\sqrt{\sum_{\text{path}} \prod_{e \in \text{path}} w(e)^2}$

- What is the relevant “complexity measure” (eg norm)?
- How is this minimized (or controlled) by the optimization algorithm?
- How does it change if we change the opt algorithm?
Where is the Regularization?

- What we did: minimize unregularized error to convergence

- In convex models, we understand how one-pass SGD (or with early stopping) provides for implicit $\ell_2$ regularization
  - More generally, Mirror Descent provides generalization w.r.t. any* inductive bias [S Sridharan Tewar, On the Universality of Mirror Descent, NIPS’11]
  - Inductive Bias $\Leftrightarrow$ choice of potential for Mirror Descent

- Here: implicit regularization, without early stopping, and even with deterministic optimization

- In underdetermined problem (lots of global optima), optimization is biasing us toward specific global optimum.

Different optimization algorithm
- Different Bias
- Different generalization properties
Cross-Entropy Training Loss

0/1 Training Error

0/1 Test Error

With Dropout

MNIST

CIFAR-10

SVHN

CIFAR-100

Epoch

[Path-SGD]

SGD

Neyshabur Salakhudtinov S NIPS’15
SGD vs ADAM

Results on Penn Treebank using 3-layer LSTM

Simple Example: Least Squares

• Consider an under-constraint least-squares problem \((n < m)\):
  \[
  \min_{w \in \mathbb{R}^n} \| A w - b \|^2
  \]
  \[A \in \mathbb{R}^{m \times n}\]

• Claim: Gradient Descent (or SGD, or conjugate gradient descent, or BFGS) converges to the least norm solution
  \[
  \min_{A w = b} \| w \|_2
  \]
  ➢ Proof: iterates always spanned by rows of \(A\) (more details soon)
reality
Section 1: Introduction
We suggest a new amazing architecture and loss function that is great for learning. All you have to do to learn is fit the model on your training data.

Section 2: Learning Contribution: our model
The model class $h_w$ is amazing. Our learning method is:

$$\arg \min_w \frac{1}{m} \sum_{i=1}^{m} \text{loss}(h_w(x); y)$$

(*)

Section 3: Optimization
This is how we solve the optimization problem (*): [...]

Section 4: Experiments
It works!
Different optimization algorithm
  ➔ Different bias in optimum reached
    ➔ Different Inductive bias
      ➔ Different generalization properties
To Understand Deep Learning

- **Ultimate Question**: What is the true Inductive Bias? What makes reality *efficiently* learnable by fitting a huge (infinite) neural net with a specific algorithm?

- **The “complexity measure” approach**: identify $c(h)$ s.t.
  - Reality is well explained by low $c(h)$
  - $\mathcal{H}_{c(\text{reality})} = \{ h | c(h) \leq c(\text{reality}) \}$ has low capacity
  - Opt. algorithm (with or w/o regularization?) biases towards low $c(h)$

- Mathematical questions:
  - What is the capacity (≡sample complexity) of the sublevel sets $\mathcal{H}_c$?
  - What is the bias of optimization algorithms?

- Question about reality (scientific Q?): does it have low $c(h)$?

- Alternative empirical questions:
  - Do models we actually learn have low $c(h)$?
  - Does it explain generalization?
  - Can we at least corelate generalization with $c(h)$?
Unconstrained Matrix Completion

\[
\min_{X \in \mathbb{R}^{n \times n}} \| \text{observed}(X) - y \|^2_2 \equiv \min_{U, V \in \mathbb{R}^{n \times n}} \| \text{observed}(UV^\top) - y \|^2_2
\]

- Underdetermined non-sensical problem, lots of useless global min
- Since \( U, V \) full dim, no constraint on \( X \), all the same non-sense global min

What happens when we optimize by gradient descent on \( U, V \)?

[Gunasekar Woodworth Bhojanapalli Neyshabur S 2017]
Gradient descent on $f(U, V)$ gets to "good" global minima

$n = 50$, $m = 300$, $A_i$ iid Gaussian, $X^*$ rank-2 ground truth $y = A(X^*) + \mathcal{N}(0, 10^{-3})$, $y_{test} = A_{test}(X^*) + \mathcal{N}(0, 10^{-3})$
Gradient descent on $f(U, V)$ gets to “good” global minima

Gradient descent on $f(U, V)$ generalizes better with smaller step size

$n = 50$, $m = 300$, $A_i$ iid Gaussian, $X^*$ rank-2 ground truth

$y = A(X^*) + \mathcal{N}(0, 10^{-3})$, $\hat{y}_{test} = A_{test}(X^*) + \mathcal{N}(0, 10^{-3})$
Grad Descent on $U, V \rightarrow \text{min nuclear norm solution}$

$$\arg \min \| X \|_* \quad s.t. \quad \text{obs}(X) = y$$

(with inf. small stepsize and initialization, exact and rigorous under additional conditions)

$\rightarrow$ good generalization if $Y$ (aprox) low rank
**Conjecture:** With stepsize→0 (i.e. gradient flow) and initialization→0, (and additional conditions?) gradient descent on $U$ converges (approximately) to minimum nuclear norm solution:

$$UU^T \rightarrow \min_{W \succeq 0} \|W\|_* \text{ s.t. } \mathcal{A}(X) = y$$

[Gunasekar Woodworth Bhojanapalli Neyshabur S 2017]

- Rigorous proof of exact convergence:
  - when $A_i$'s commute
  - [Yuanzhi Li, Hongyang Zhang and Tengyu Ma, COLT 2018]:
    when $y = \mathcal{A}$ (low rank $W^*$), $\mathcal{A}$ RIP

- General $A_i$: empirical validation (approximate) + hand waving
Understand optimization algorithm not just as reaching *some* (global) optimum, but as reaching a *specific* optimum.
Implicit Bias in Least Squared

\[ \min ||Aw - b||^2 \]

- Gradient Descent (+Momentum) on \( w \)
  \[ \Rightarrow \min_{Aw=b} ||w||_2 \]
- Gradient Descent on factorization \( W = UV \)
  \[ \Rightarrow \text{probably } \min_{A(W)=b} \|W\|_{tr} \text{ with stepsize} \downarrow 0 \text{ and init} \downarrow 0, \]
  but only in limit, depends on stepsize, init, proved only in special cases
- AdaGrad on \( w \)
  \[ \Rightarrow \text{in some special cases } \min_{Aw=b} ||w||_\infty, \text{ but not always,} \]
  and it depends on stepsize, adaptation param, momentum
- Steepest Descent w.r.t. \( ||w|| \)
  \[ \Rightarrow \text{??? Not } \min_{Aw=b} ||w||, \text{ even as stepsize} \downarrow 0 ! \]
  and it depends on stepsize, init, momentum
- Coordinate Descent (steepest descent w.r.t. \( ||w||_1 \))
  \[ \Rightarrow \text{Related to, but not quite the Lasso} \]
  (with stepsize \( \downarrow 0 \) and particular tie-breaking \( \approx \) LARS)
Implicit Bias in Logistic Regression

\[
\arg \min_{w \in \mathbb{R}^n} \mathcal{L}(w) = \sum_{i=1}^{m} \ell(y_i \langle w, x_i \rangle)
\]

\[
\ell(z) = \log(1 + e^{-z})
\]

- Data \(\{(x_i, y_i)\}_{i=1}^m\) linearly separable (\(\exists w \forall i y_i \langle w, x_i \rangle > 0\))
- Where does gradient descent converge?
  \[
  w(t) = w(t) - \eta \nabla \mathcal{L}(w(t))
  \]
  - \(\inf \mathcal{L}(w) = 0\), but minima unattainable
  - GD diverges to infinity: \(w(t) \to \infty, \mathcal{L}(w(t)) \to 0\)
- **In what direction?** What does \(\frac{w(t)}{\|w(t)\|}\) converge to?
Implicit Bias in Logistic Regression

\[
\arg \min_{w \in \mathbb{R}^n} \mathcal{L}(w) = \sum_{i=1}^{m} \ell(y_i \langle w, x_i \rangle)
\]

\[
\ell(z) = \log(1 + e^{-z})
\]

- Data \(\{(x_i, y_i)\}_{i=1}^{m}\) linearly separable (\(\exists w \forall i \ y_i \langle w, x_i \rangle > 0\))
- Where does gradient descent converge?
  \[
w(t) = w(t) - \eta \nabla \mathcal{L}(w(t))
\]
  - inf \(\mathcal{L}(w) = 0\), but minima unattainable
  - GD diverges to infinity: \(w(t) \to \infty, \mathcal{L}(w(t)) \to 0\)
- **In what direction?** What does \(\frac{w(t)}{\|w(t)\|}\) converge to?
- **Theorem:** \(\frac{w(t)}{\|w(t)\|_2} \to \frac{\hat{w}}{\|\hat{w}\|_2}\) \(\hat{w} = \arg \min \|w\|_2 \ s.t. \ \forall i \ y_i \langle w, x_i \rangle \geq 1\)
Logistic Regression on Separable Data

$$\arg \min_{w \in \mathbb{R}^n} \mathcal{L}(w) = \sum_{i=1}^{m} \ell(y_i \langle w, x_i \rangle)$$

$$\ell(z) = \log(1 + e^{-z})$$

**Theorem:** \( \frac{w(t)}{\|w(t)\|_2} \rightarrow \frac{\hat{w}}{\|\hat{w}\|_2} \) \quad \hat{w} = \arg \min \|w\|_2 \quad s.t. \quad \forall_i y_i \langle w, x_i \rangle \geq 1

- \( w(t) = \hat{w} \log t + \rho(t) \), with \( \rho(t) \) bounded*
- Holds for any initial point \( w(0) \) and stepsize \( \eta \leq 2 \)
- Holds for any monotonically decreasing strictly positive smooth loss s.t. 
  - \( \ell'(z) \) has a tight exponential tail

*For data in general position. With degenerate data, \( \rho(t) = O(\log \log t) \)
**Proof sketch:** ($y_i = 1$ w.l.o.g.)

Write $w(t) = g(t)w_\infty + \rho(t)$ with $g(t) \to \infty$ and $\rho(t) = o(g(t))$.

Since we converge to zero error, $\forall_i \langle w_\infty, x_i \rangle > 0$

Since the loss derivative has an exponential tail:

$$-\nabla \mathcal{L}(w) \approx \sum_i e^{-\langle w(t), x_i \rangle} x_i^T = \sum_i e^{-g(t)\langle w_\infty, x_i \rangle - \langle \rho(t), x_i \rangle} x_i^T$$

As $g(t) \to \infty$, only points with minimal $\langle w_\infty, x_i \rangle$ (points on the margin, "support vectors") will dominate gradient

$\Rightarrow \nabla \mathcal{L}(w)$ spanned by support vectors

$\Rightarrow w(t)$ spanned by support vectors

Define $\hat{w} = \frac{w_\infty}{\min_i \langle w_\infty, x_i \rangle}$. We have:

$$\hat{w} = \sum \alpha_i w_i \quad \forall_i (\alpha_i \geq 0 \text{ and } \langle \hat{w}, x_i \rangle = 1) \text{ OR } (\alpha_i = 0 \text{ and } \langle \hat{w}, x_i \rangle > 1)$$
How Fast is the Margin Maximized?

Convergence to the max margin $\hat{w}$: *

$$\left\| \frac{w(t)}{\|w(t)\|} - \frac{\hat{w}}{\|\hat{w}\|} \right\| = O\left( \frac{1}{\log t} \right)$$

Convergence of the margin itself:

$$\max_{\|w\| \leq 1} \min_i y_i \langle w, x_i \rangle - \min_i y_i \left( \frac{w(t)}{\|w(t)\|}, x_i \right) = O\left( \frac{1}{\log t} \right)$$

Contrast with convergence of the loss:

$$\mathcal{L}(w(t)) = O\left( \frac{1}{t} \right)$$

⇒ Even after we get extremely small loss, need to continue optimizing in order to maximize margin

*For data in general position. With degenerate data, $O(\log \log t / \log t)$
Training a conv net using SGD+momentum on CFAIR10
Other Objectives and Opt Methods

• Single linear unit, logistic loss
  ➔ hard margin SVM solution (regardless of init, stepsize)

• Multi-class problems with softmax loss
  ➔ multiclass SVM solution (regardless of init, stepsize)

• Steepest Descent w.r.t. $\|w\|$ 
  ➔ $\arg\min \|w\| \text{ s.t. } \forall y_i \langle w, x_i \rangle \geq 1$ (regardless of init, stepsize)

• Coordinate Descent
  ➔ $\arg\min \|w\|_1 \text{ s.t. } \forall y_i \langle w, x_i \rangle \geq 1$ (regardless of init, stepsize)

• Matrix factorization problems $\mathcal{L}(U, V) = \sum_i \ell(\langle A_i, UV^T \rangle)$, including 1-bit matrix completion 
  ➔ $\arg\min \|W\|_{tr} \text{ s.t. } \langle A_i, W \rangle \geq 1$ (regardless of init)
Different Asymptotics

• For least squares (or any other loss with attainable minimum):
  • $w_\infty$ depends on initial point $w_0$ and stepsize $\eta$
  • To get clean characterization, need to take $\eta \to 0$
  • If $0$ is a saddle point, need to take $w_0 \to 0$

• For monotone decreasing loss (eg logistic)
  • $w_\infty$ does NOT depend on initial $w_0$ and stepsize $\eta$
  • Don’t need $\eta \to 0$ and $w_0 \to 0$
  • What happens at the beginning doesn’t effect $w_\infty$
Single Overparametrized Linear Unit

Train single unit with SGD using logistic ("cross entropy") loss
→ **Hard Margin SVM predictor**
\[ w(\infty) \propto \arg\min_{w} \|w\|_2 \quad s.\ t. \quad \forall \ y_i \langle w, x_i \rangle \geq 1 \]

Even More Overparameterization: Deep Linear Networks

Network implements a linear mapping:
\[ f_w(x) = \langle \beta_w, x \rangle \]
Training: same opt. problem as logistic regression:
\[ \min_w \mathcal{L}(f_w) \equiv \min_\beta \mathcal{L}(x \mapsto \langle \beta, x \rangle) \]

Train \( w \) with SGD
→ **Hard Margin SVM predictor**
\[ \beta_{w(\infty)} \rightarrow \arg\min_{\beta} \|\beta\|_2 \quad s.\ t. \quad \forall \ y_i \langle \beta, x_i \rangle \geq 1 \]
L-1 hidden layers, $h_l \in \mathbb{R}^n$, each with (one channel) full-width cyclic “convolution” $w_\ell \in \mathbb{R}^D$:

$$h_l[d] = \sum_{k=0}^{D-1} w_\ell[k]h_{l-1}[d + k \text{ mod } D] \quad h_{out} = \langle w_L, h_{L-1} \rangle$$

With single conv layer (L=2), training weights with SGD

$$\rightarrow \arg\min \|DFT(\beta)\|_1 \text{ s.t. } \forall y_i \langle \beta, x_i \rangle \geq 1$$

With multiple conv layers

$$\rightarrow \text{critical point of } \min \|DFT(\beta)\|_{2/L} \text{ s.t. } \forall y_i \langle \beta, x_i \rangle \geq 1$$

for $\ell(z) = \exp(-z)$, almost all linearly separable data sets and initializations $w(0)$ and any bounded stepsizes s.t. $\mathcal{L} \to 0$, and $\Delta w(t)$ converge in direction

[Gunasekar Lee Soudry S 2018]
$$\min \| \beta \|_2 \quad s.t. \quad \forall i \ y_i \langle \beta, x_i \rangle \geq 1$$

$$\min \frac{\| DFT(\beta) \|_2}{L} \quad s.t. \quad \forall i \ y_i \langle \beta, x_i \rangle \geq 1$$

$$\min \| \beta \|_2 / L \quad s.t. \quad \forall i \ y_i \langle \beta, x_i \rangle \geq 1$$
Effect of Parametrization

• Matrix completion (also: reconstruction from linear measurements)
  • $X = UV$ is over-parametrization of all matrices $X \in \mathbb{R}^{n \times n}$
  • GD on $U, V \Rightarrow$ implicitly minimize $\|X\|_*$

  [Gunasekar Woodworth Bhojanapalli Neyshabur S 2017]

• Linear Convolutional Network:
  • Complex over-parametrization of linear predictors $\beta$
  • GD on weight $\Rightarrow$ implicitly minimize $\|DFT(\beta)\|_p$ for $p = \frac{2}{\text{depth}}$.
    (sparsity in frequency domain)

  [Gunasekar Lee Soudry S 2018]

• Infinite Width ReLU Net with 1-d input:
  • Parametrization of essentially all functions $f : \mathbb{R} \to \mathbb{R}$
  • Weight decay $\Rightarrow$ implicitly minimize...
    $$\max \left( \int |f''| dx, |f'(-\infty) + f'(+\infty)| \right)$$

  [Savarese Evron Soudry S 2019]
Optimization Geometry and hence Inductive Bias effected by:

- Geometry of local search in parameter space
- Choice of parameterization
To Understand Deep Learning

**Ultimate Question:** What is the true Inductive Bias? What makes reality *efficiently* learnable by fitting a huge (infinite) neural net with a specific algorithm?

**The “complexity measure” approach:** identify $c(h)$ s.t.
- Reality is well explained by low $c(h)$
- $\mathcal{H}_{c(\text{reality})} = \{h| c(h) \leq c(\text{reality})\}$ has low capacity
- Opt. algorithm (with or w/o regularization?) biases towards low $c(h)$

**Mathematical questions:**
- What is the capacity (≡sample complexity) of the sublevel sets $\mathcal{H}_c$?
- **What is the bias of optimization algorithms?**

**Question about reality (scientific Q?):** does it have low $c(h)$?

**Alternative empirical questions:**
- Do models we actually learn have low $c(h)$?
- Does it explain generalization?
- Can we at least correlate generalization with $c(h)$?