Optimization for Machine Learning

Introduction into supervised learning, stochastic gradient descent analysis and tricks

Lecturer: Robert M. Gower

TELECOM ParisTech

28^{th} of April to 5^{th} of May 2020, Cornell mini-lecture series, online

Outline of my three classes

- 04/27/20 Intro to empirical risk problem and stochastic gradient descent (SGD)
- 04/29/20 SGD for convex optimization. Theory and variants
- 05/05/20 SGD with momentum and tricks

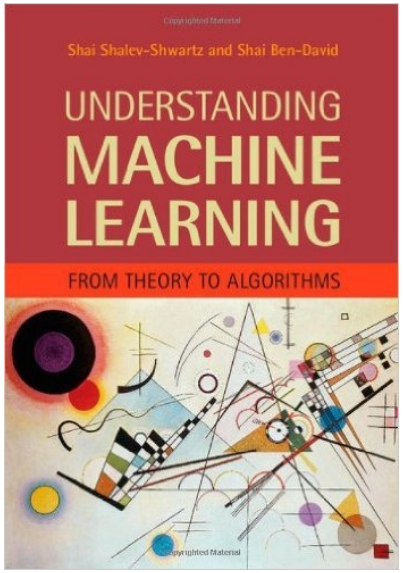
Part I: An Introduction to Supervised Learning

References classes today

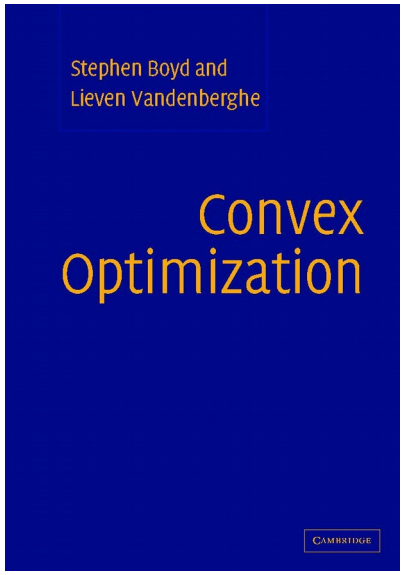
Chapter 2

Pages 67 to 79

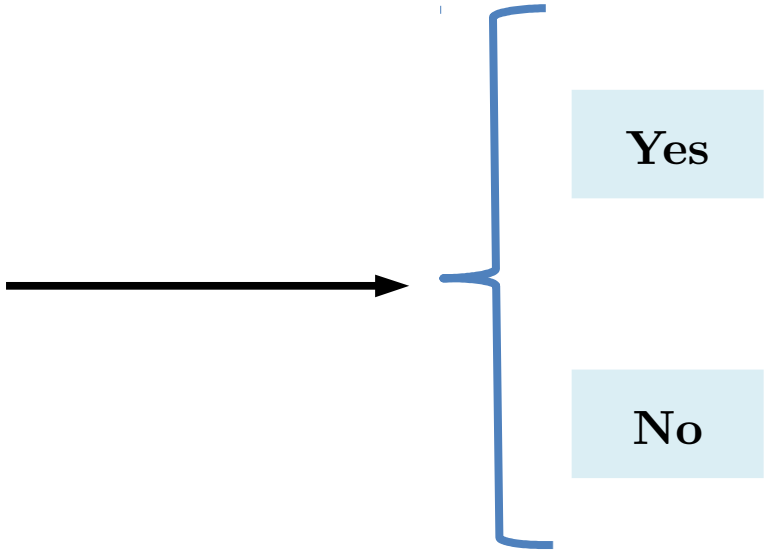
Understanding Machine Learning: From Theory to Algorithms



Convex Optimization, Stephen Boyd



Is There a Cat in the Photo?



Is There a Cat in the Photo?

Yes

Is There a Cat in the Photo?

Yes

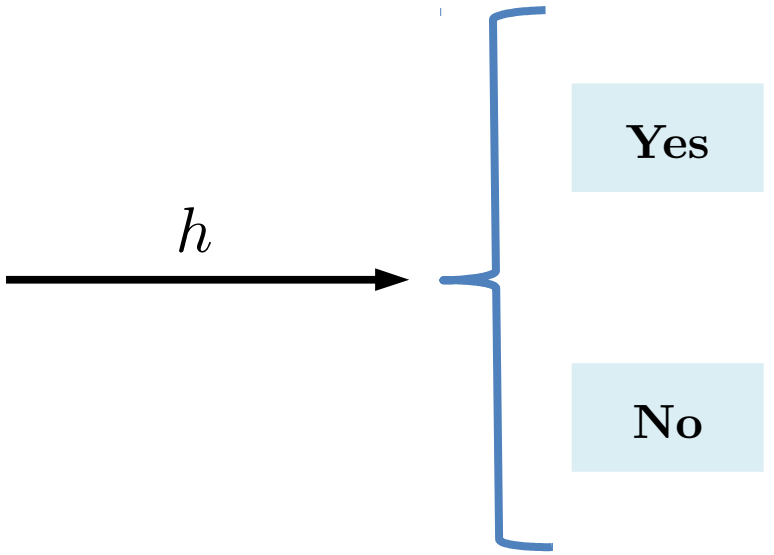
Is There a Cat in the Photo?

No

Is There a Cat in the Photo?

Yes

Is There a Cat in the Photo?



x: Input/Feature

y: Output/Target

Find mapping h that assigns the "correct" target to each input

$$h : x \in \mathbf{R}^d \longrightarrow y \in \mathbf{R}$$

Labeled Data: The training set

x^1 {  $y^1 = 1$

x^2 {  $y^2 = 1$

x^3 {  $y^3 = -1$

$\cdots$ x^n {  $y^n = 1$

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Training Algorithm

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Training Algorithm

$h : x \in \mathbf{R}^d \rightarrow y \in \mathbf{R}$

h ()

-1

Example: Linear Regression for Height

Male = 0
Female = 1

Labelled data $x \in \mathbf{R}^2, y \in \mathbf{R}_+$

x_1^1	Sex	0		x_1^n	Sex	1
x_2^1	Age	30	$\cdots$	x_2^n	Age	70
y^1	Height	1,72 cm		y^n	Height	1,52 cm

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Example Hypothesis: Linear Model

$$h_w(x_1, x_2) = w_0 + x_1 w_1 + x_2 w_2 \overset{x_0=1}{=} \langle w, x \rangle$$

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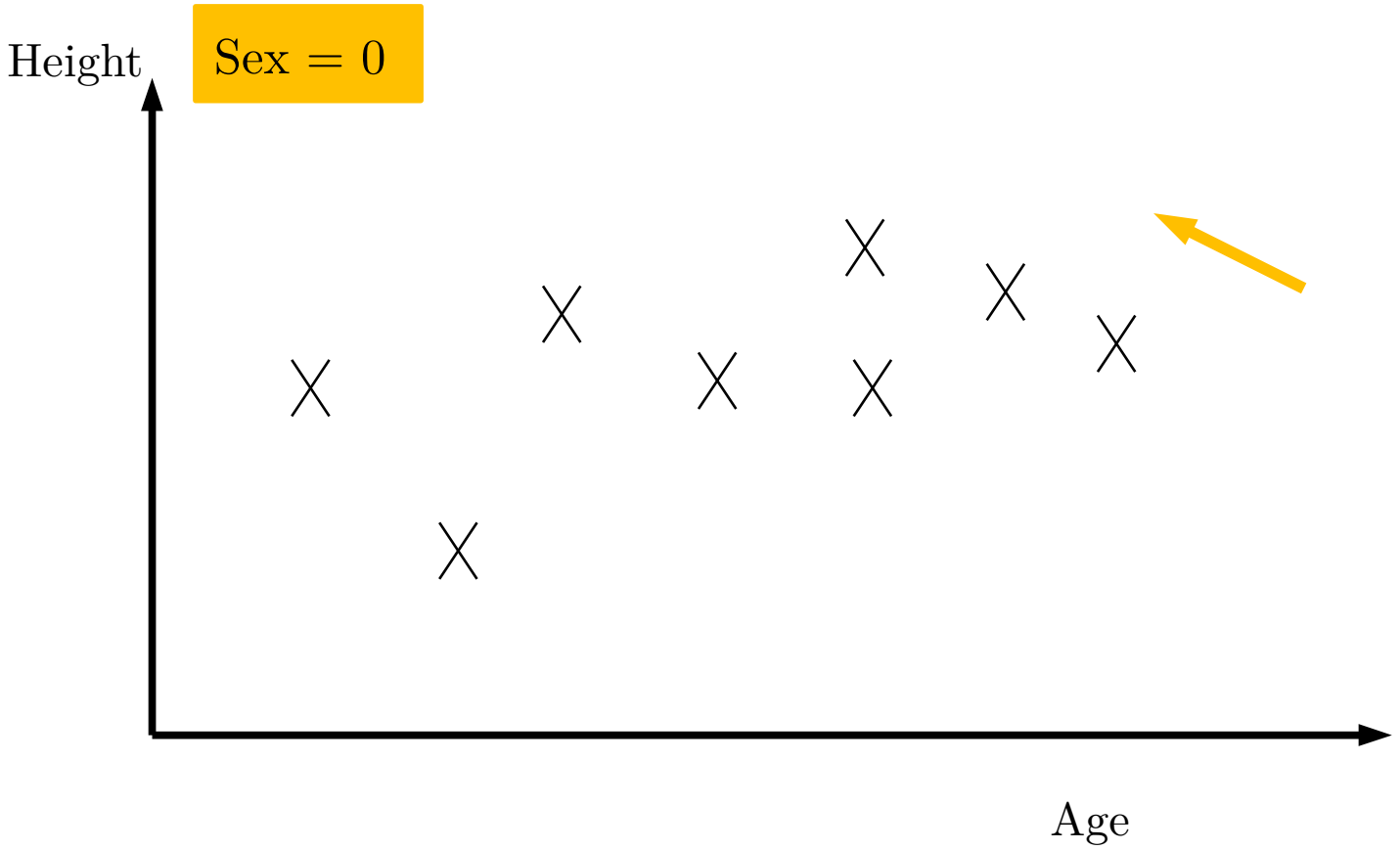
Example Training Problem:

$$\min_{w \in \mathbf{R}^3} \frac{1}{n} \sum_{i=1}^{n} \left(h_w(x_1^i, x_2^i) - y^i \right)^2$$

Linear Regression for Height



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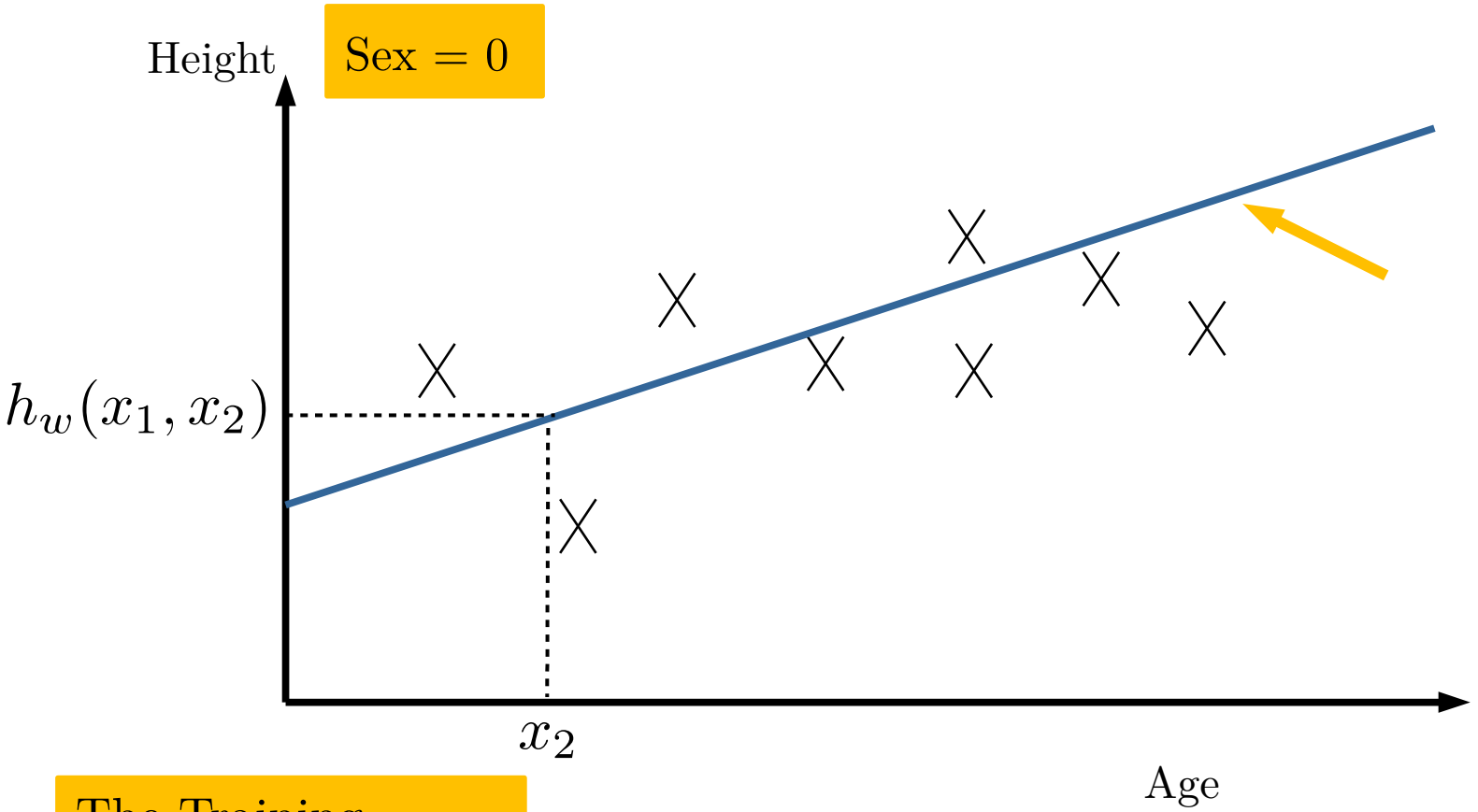
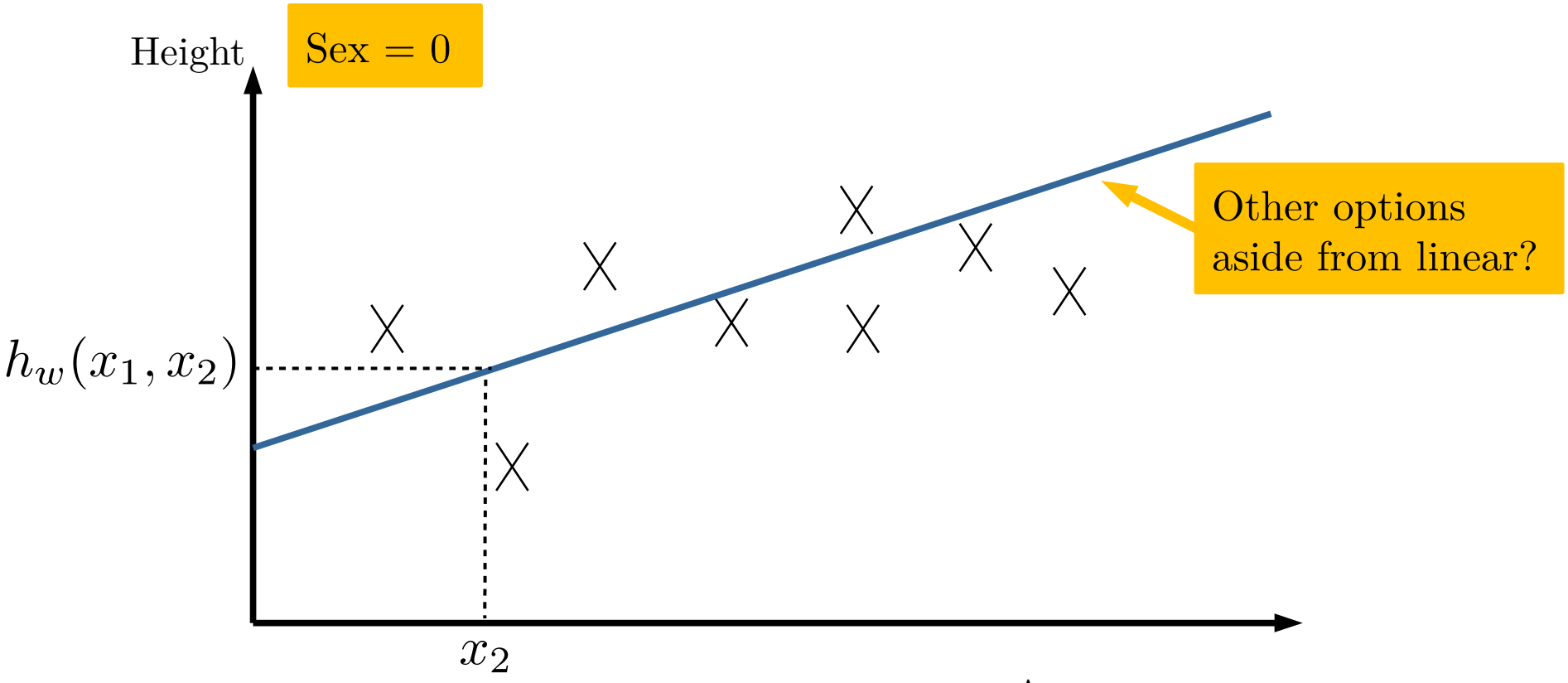


The Training Algorithm

$$\min_{w \in \mathbf{R}^3} \frac{1}{n} \sum_{i=1}^{n} \left(h_w(x_1^i, x_2^i) - y^i \right)^2$$

Linear Regression for Height



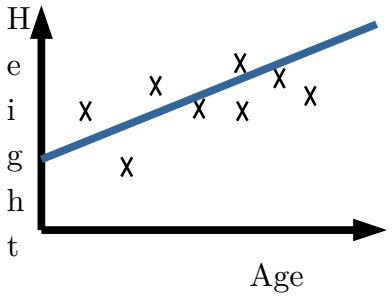
The Training Algorithm

$$\min_{w \in \mathbf{R}^3} \frac{1}{n} \sum_{i=1}^{n} \left(h_w(x_1^i, x_2^i) - y^i \right)^2$$

Parametrizing the Hypothesis

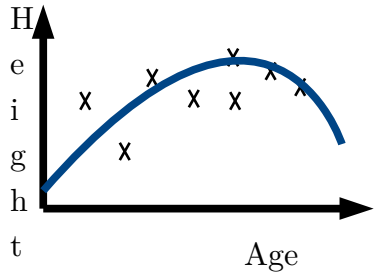
Linear:

$$h_w(x) = \sum_{i=0}^{d} w_i x_i$$

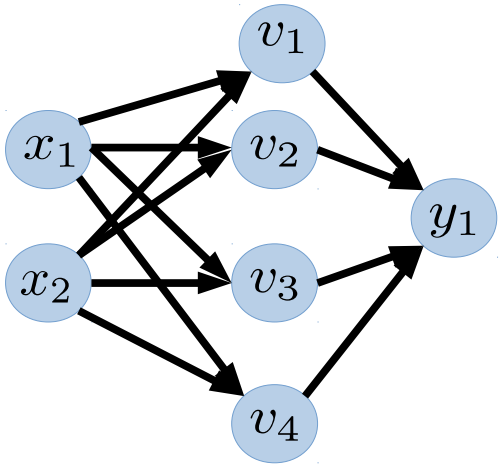


Polinomial:

$$h_w(x) = \sum_{i,j=0}^{d} w_{ij} x_i x_j$$



Neural Net:



exe :

$$v_1 = \text{sign}(w_{11}x_1 + w_{12}x_2)$$

$$v_4 = 1/\left(1 + \exp(w_{41}x_1 + w_{42}x_2)\right)$$

Loss Functions

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \left(h_w(x^i) - y^i \right)^2$$

Why a Squared Loss?

Loss Functions

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \left(h_w(x^i) - y^i \right)^2$$

Why a Squared Loss?

Let $y_h := h_w(x)$

Loss Functions

$$\begin{array}{rccc} \ell: & \mathbf{R} \times \mathbf{R} & \rightarrow & \mathbf{R}_+ \\ & (y_h, y) & \rightarrow & \ell(y_h, y) \end{array}$$

The Training Problem

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \ell \left(h_w(x^i), y^i \right)$$

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Typically a convex function

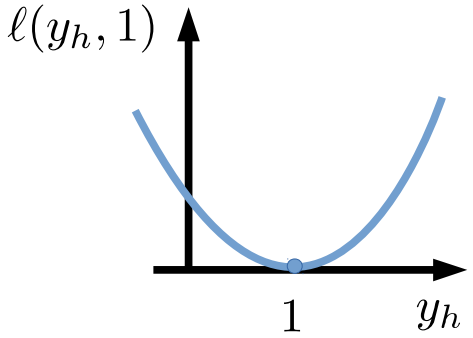
The Training Problem

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \ell \left(h_w(x^i), y^i \right)$$

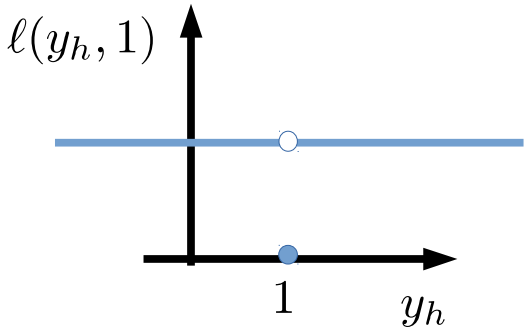
Choosing the Loss Function

Let $y_h := h_w(x)$

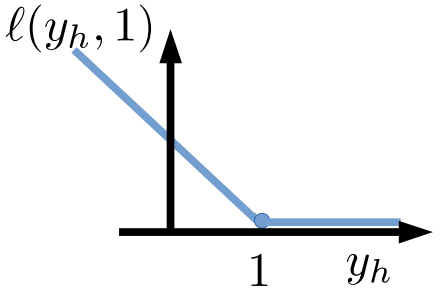
Quadratic Loss $\ell(y_h, y) = (y_h - y)^2$



Binary Loss $\ell(y_h, y) = \begin{cases} 0 & \text{if } y_h = y \\ 1 & \text{if } y_h \neq y \end{cases}$



Hinge Loss $\ell(y_h, y) = \max\{0, 1 - y_h y\}$



Choosing the Loss Function

$y=1$ in all figures

Let $y_h := h_w(x)$

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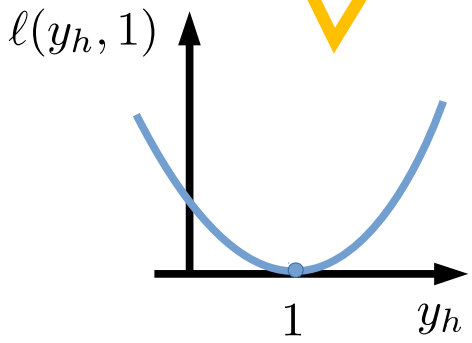

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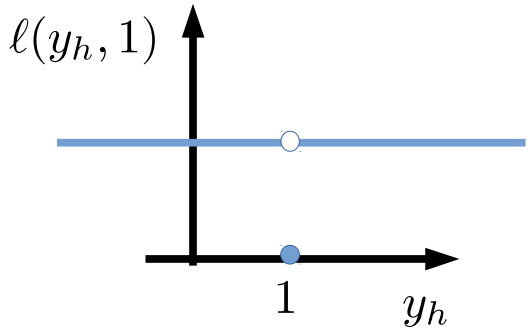

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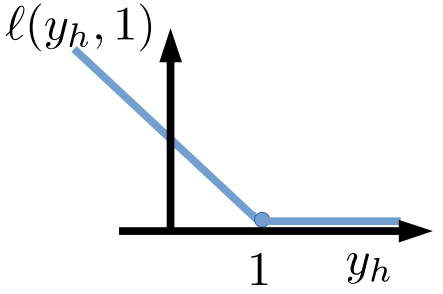

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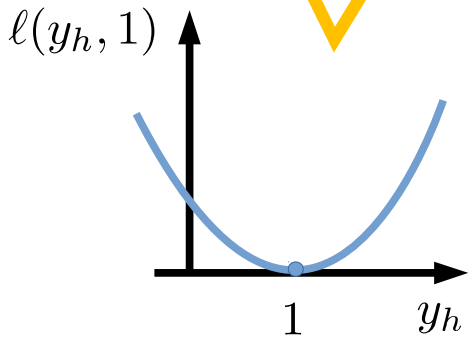

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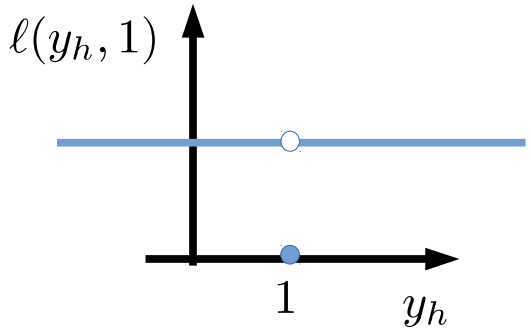

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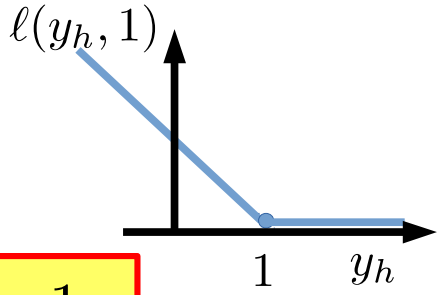


EXE: Plot the binary and hinge loss function in when $y = -1$

Loss Functions

Is a notion of Loss enough?

What happens when we do not have enough data?

Loss Functions

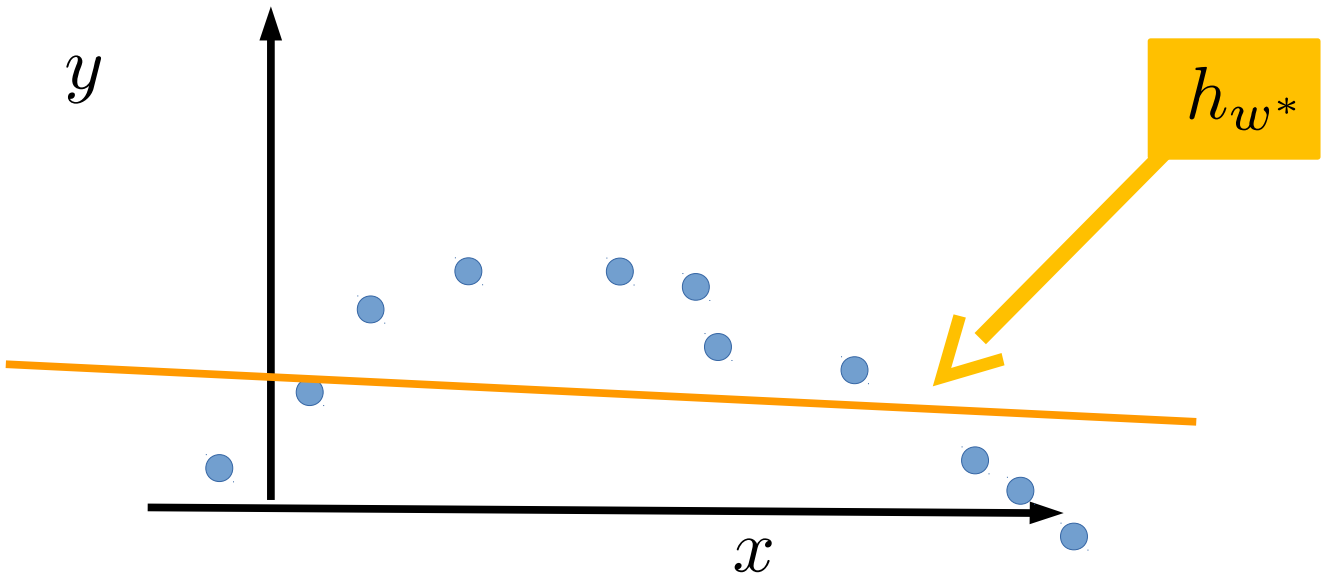
The Training Problem

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \ell\left(h_w(x^i), y^i\right)$$

Is a notion of Loss enough?

What happens when we do not have enough data?

Overfitting and Model Complexity

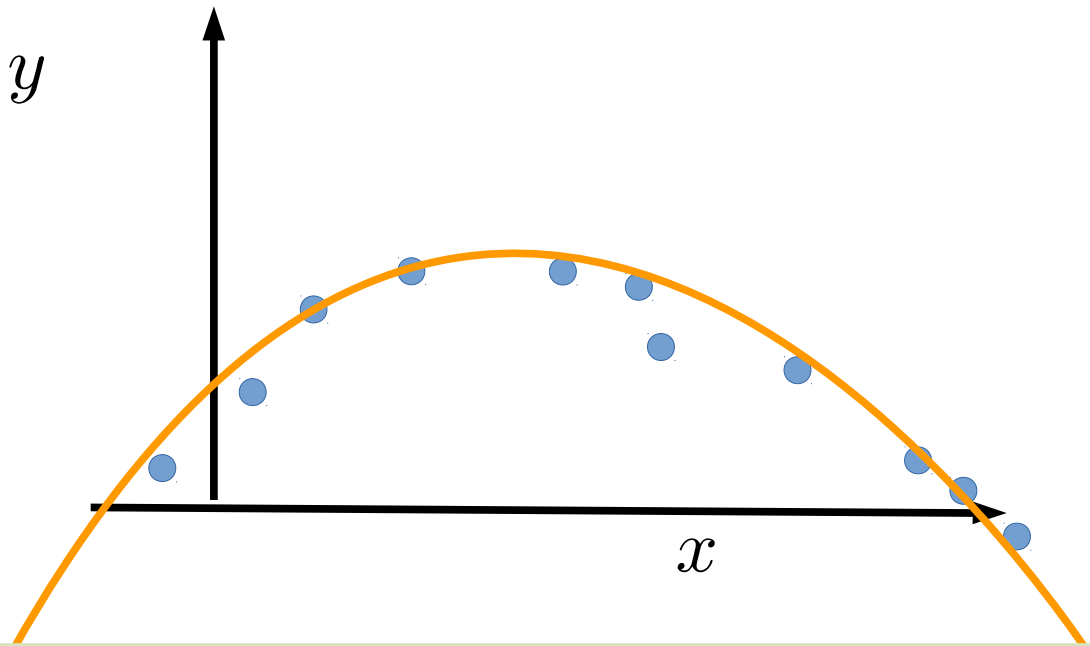


Fitting 1st order polynomial

$$h_w = \langle w, x \rangle$$

$$w^* = \arg \min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \left(h_w(x^i) - y^i \right)^2$$

Overfitting and Model Complexity

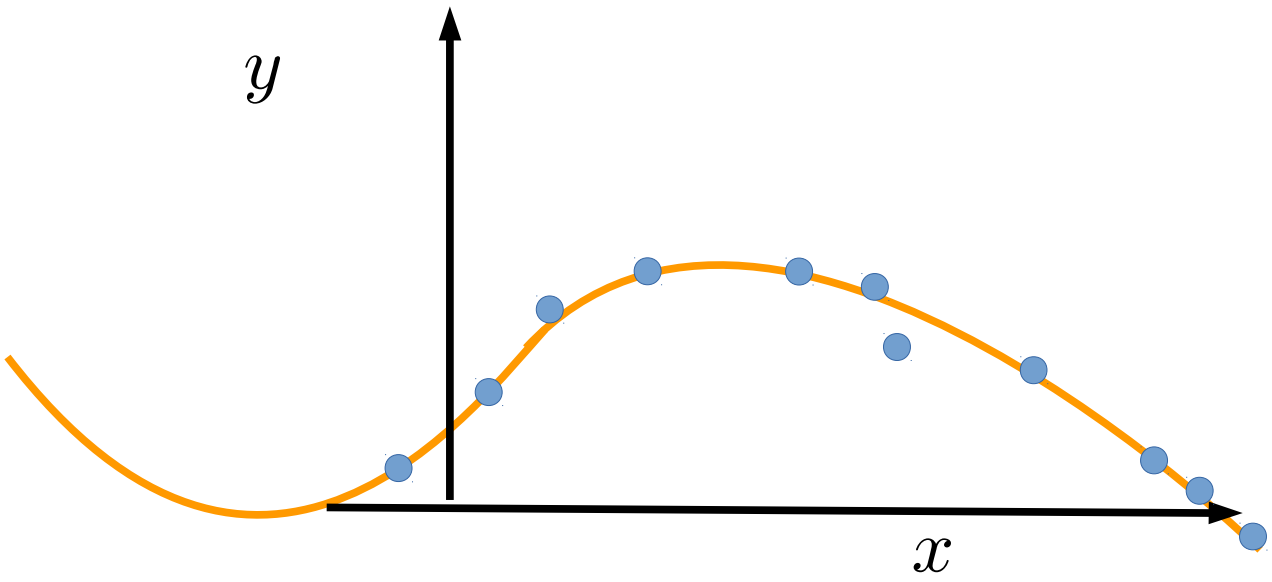


Fitting 2nd order polynomial

$$h_w = w_0 + w_1 x + w_2 x^2$$

$$w^* = \arg\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \left(h_w(x^i) - y^i \right)^2$$

Overfitting and Model Complexity



Fitting 3rd order polynomial

$$h_w = \sum_{i=0}^{3} w_i x^i$$

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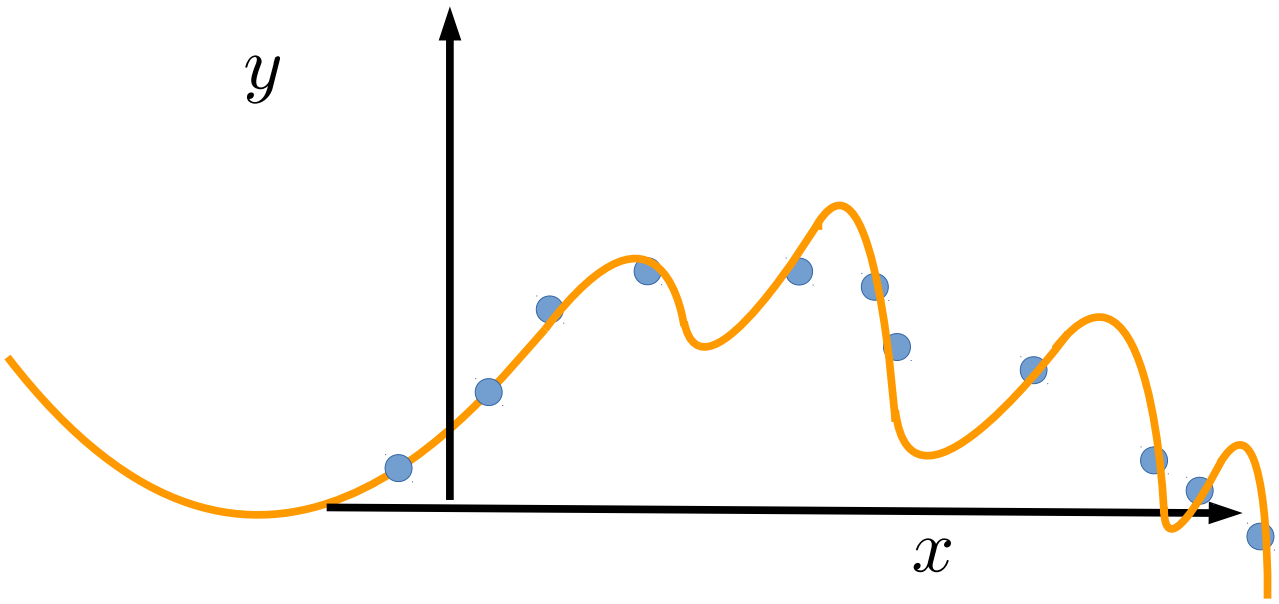
Overfitting and Model Complexity



Fitting 9^{th} order polynomial

$$h_w = \sum_{i=0}^{9} w_i x^i$$

$$w^* = \arg\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \left(h_w(x^i) - y^i \right)^2$$

Regularization

Regularizor Functions

$$\begin{array}{rccc} R: & \mathbf{R}^d & \rightarrow & \mathbf{R}_+ \\ & w & \rightarrow & R(w) \end{array}$$

General Training Problem

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \ell\left(h_w(x^i), y^i\right) + \lambda R(w)$$

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Goodness of fit,
fidelity term ...etc

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Penalizes complexity

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Controls tradeoff between fit and complexity

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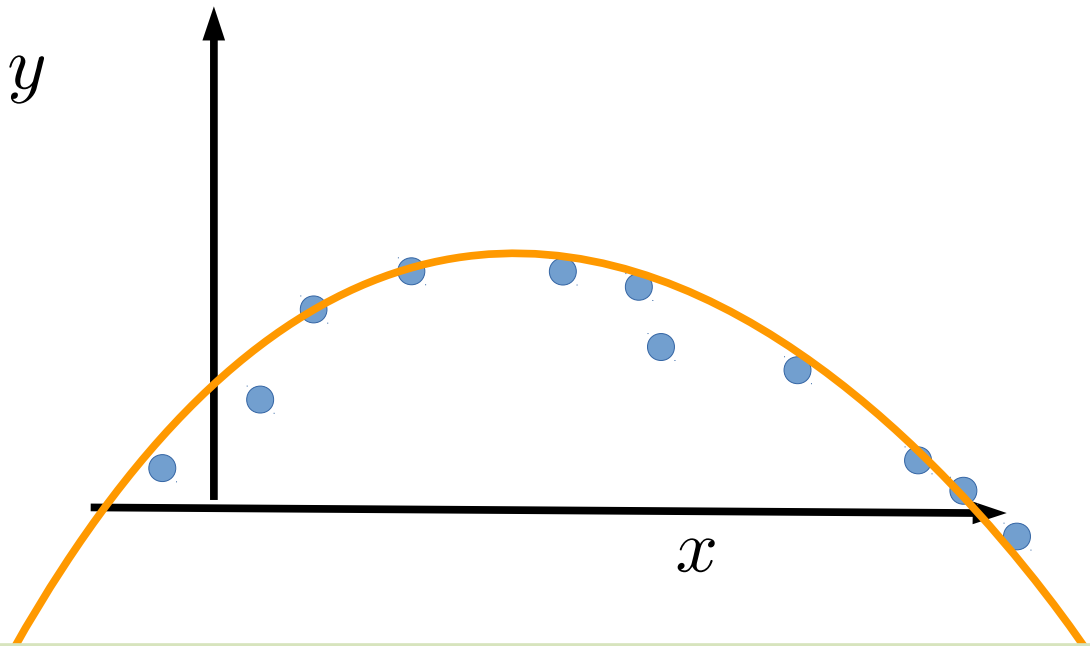
Goodness of fit, fidelity term ...etc

Penalizes complexity

Exe:

$$R(w) = ||w||_2^2, \quad ||w||_1, \quad ||w||_p, \quad \text{other norms } \ldots$$

Overfitting and Model Complexity

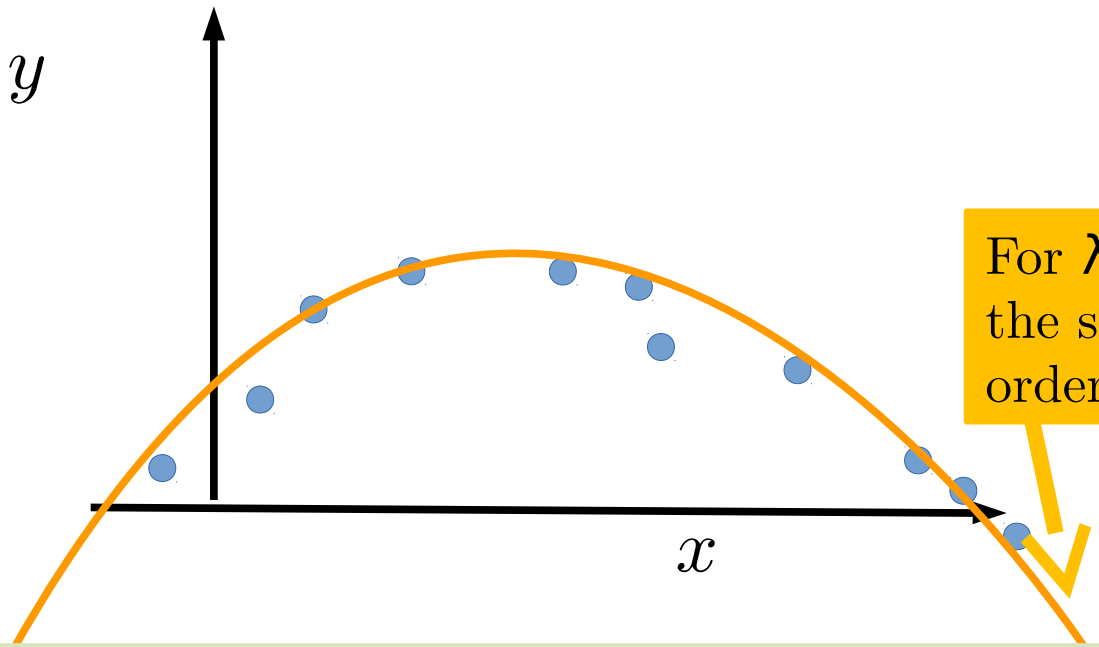


Fitting k$^{\text{th}}$ order polynomial

$$h_w = \sum_{i=0}^{k} w_i x^i$$

$$w^* = \arg\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \left(h_w(x^i) - y^i \right)^2 + \lambda ||w||_1$$

Overfitting and Model Complexity



For λ big enough, the solution is a 2nd order polynomial

Fitting k$^{\text{th}}$ order polynomial

$$h_w = \sum_{i=0}^{k} w_i x^i$$

$$w^* = \arg\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \left(h_w(x^i) - y^i \right)^2 + \lambda ||w||_1$$

Exe: Ridge Regression

Linear hypothesis

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

L2 regularizor

$$R(w) = ||w||_2^2$$

L2 loss

$$\ell(y_h, y) = (y_h - y)^2$$

Ridge Regression

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} (y^i - \langle w, x^i \rangle)^2 + \lambda ||w||_2^2$$

Exe: Support Vector Machines

Linear hypothesis

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

L2 regularizor

$$R(w) = ||w||_2^2$$

Hinge loss

$$\ell(y_h, y) = \max\{0, 1 - y_h y\}$$

SVM with soft margin

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \max\{0, 1 - y^i \langle w, x^i \rangle\} + \lambda ||w||_2^2$$

Exe: Logistic Regression

Linear hypothesis

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

L2 regularizor

$$R(w) = ||w||_2^2$$

Logistic loss

$$\ell(y_h, y) = \ln(1 + e^{-yy_h})$$

Logistic Regression

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \ln(1 + e^{-y^i \langle w, x^i \rangle}) + \lambda ||w||_2^2$$

The Machine Learners Job

(1) Get the labeled data: $(x^1, y^1), \ldots, (x^n, y^n)$

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(2) Choose a parametrization for hypothesis: $h_w(x)$

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Part II: Optimizing Empirical Risk

Re-writing as Sum of Terms

A Datum Function

$$f_i(w) := \ell\left(h_w(x^i), y^i\right) + \lambda R(w)$$

$$\begin{aligned}\frac{1}{n}\sum_{i=1}^{n} \ell\left(h_w(x^i), y^i\right) + \lambda R(w) &= \frac{1}{n}\sum_{i=1}^{n}\left(\ell\left(h_w(x^i), y^i\right) + \lambda R(w)\right) \\ &= \frac{1}{n}\sum_{i=1}^{n} f_i(w)\end{aligned}$$

Finite Sum Training Problem

$$\min_{w\in\mathbf{R}^d} \frac{1}{n}\sum_{i=1}^{n} f_i(w) =: f(w)$$

Can we use this sum structure?

The Training Problem

Solving the *training problem*:

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} f_i(w)$$

Reference method: Gradient descent

$$\nabla \left(\frac{1}{n} \sum_{i=1}^{n} f_i(w) \right) = \frac{1}{n} \sum_{i=1}^{n} \nabla f_i(w)$$

Gradient Descent Algorithm

Set $w^0 = 0$, choose $\alpha > 0$.

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

$$w^{t+1} = w^t - \frac{\alpha}{n} \sum_{i=1}^{n} \nabla f_i(w^t)$$

Output w^T

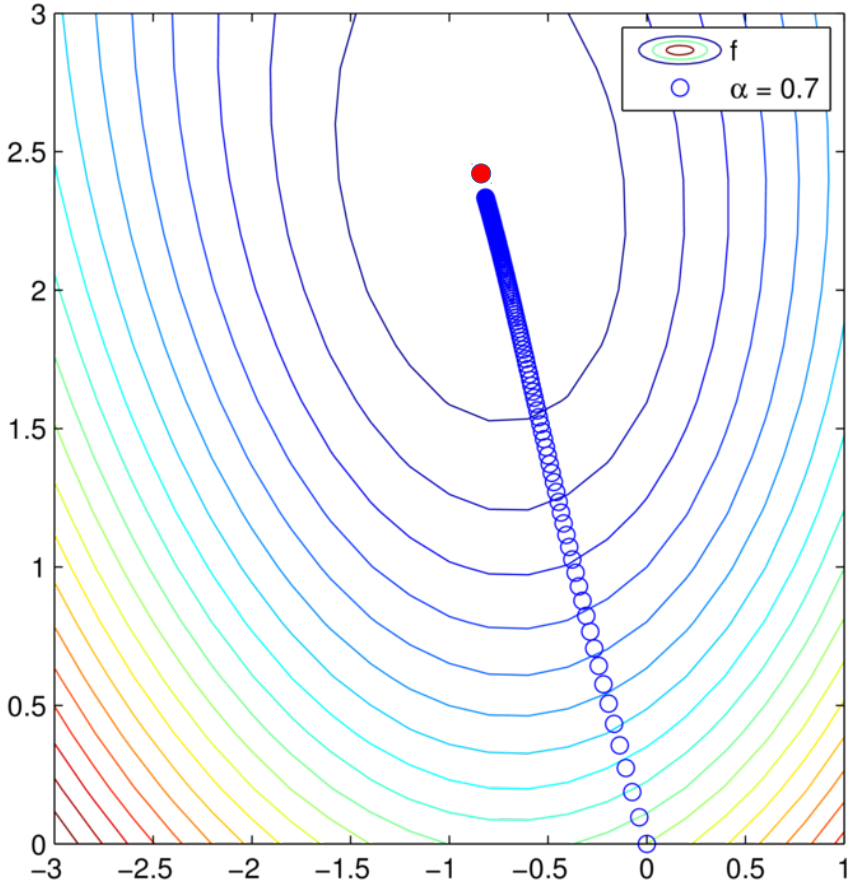
Gradient Descent Example

A Logistic Regression problem using the fourclass labelled data from LIBSVM

$(n,\ d) = (862,2)$

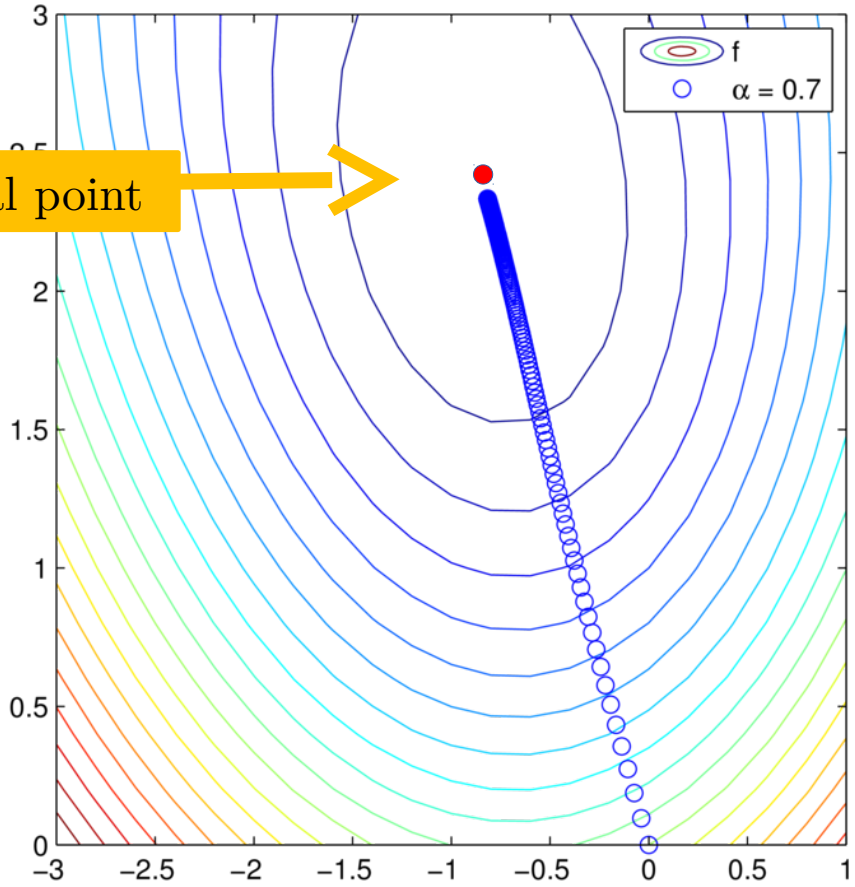
Logistic Regression

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \ln(1 + e^{-y^i \langle w, x^i \rangle}) + \lambda ||w||_2^2$$



Can we prove that this always works?

Gradient Descent Example



Optimal point

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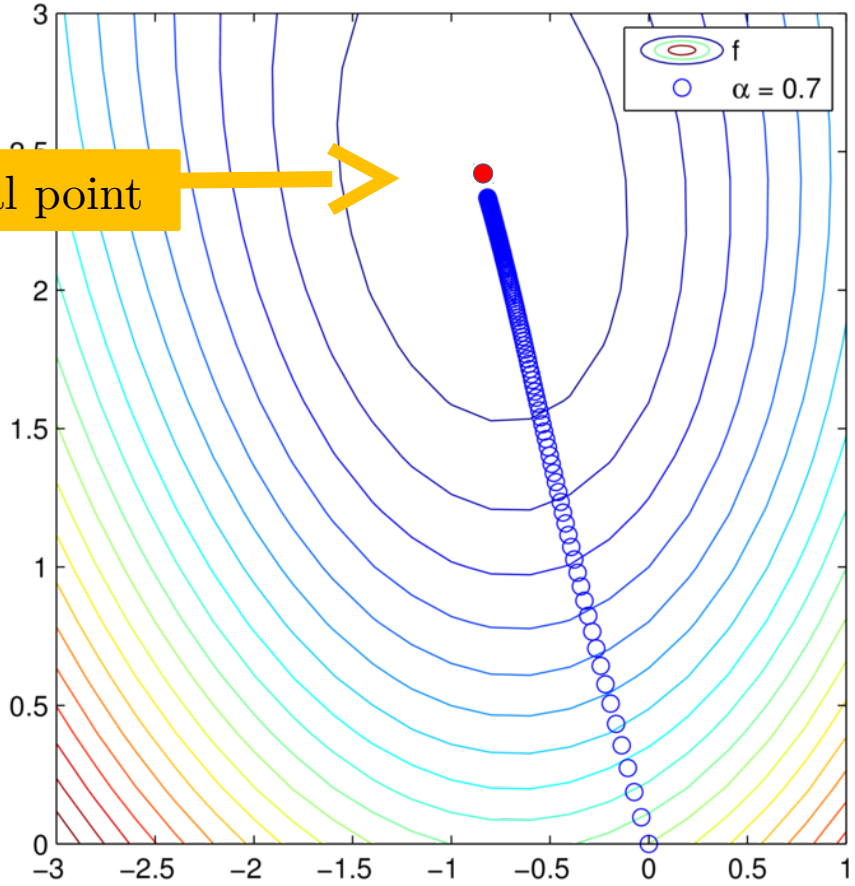

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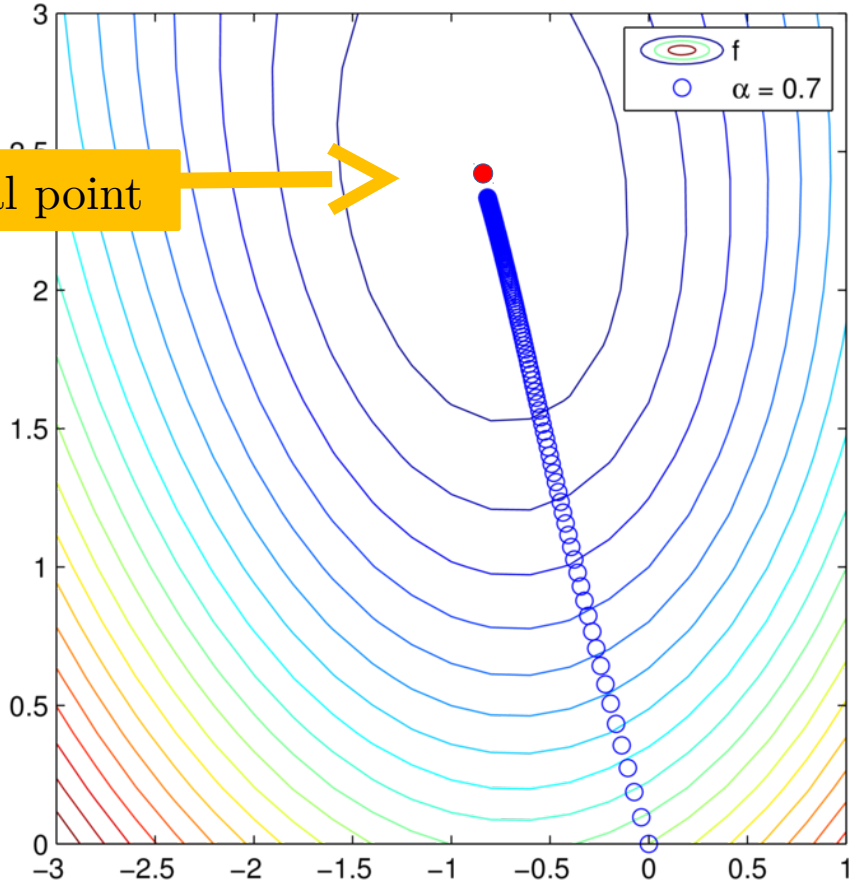

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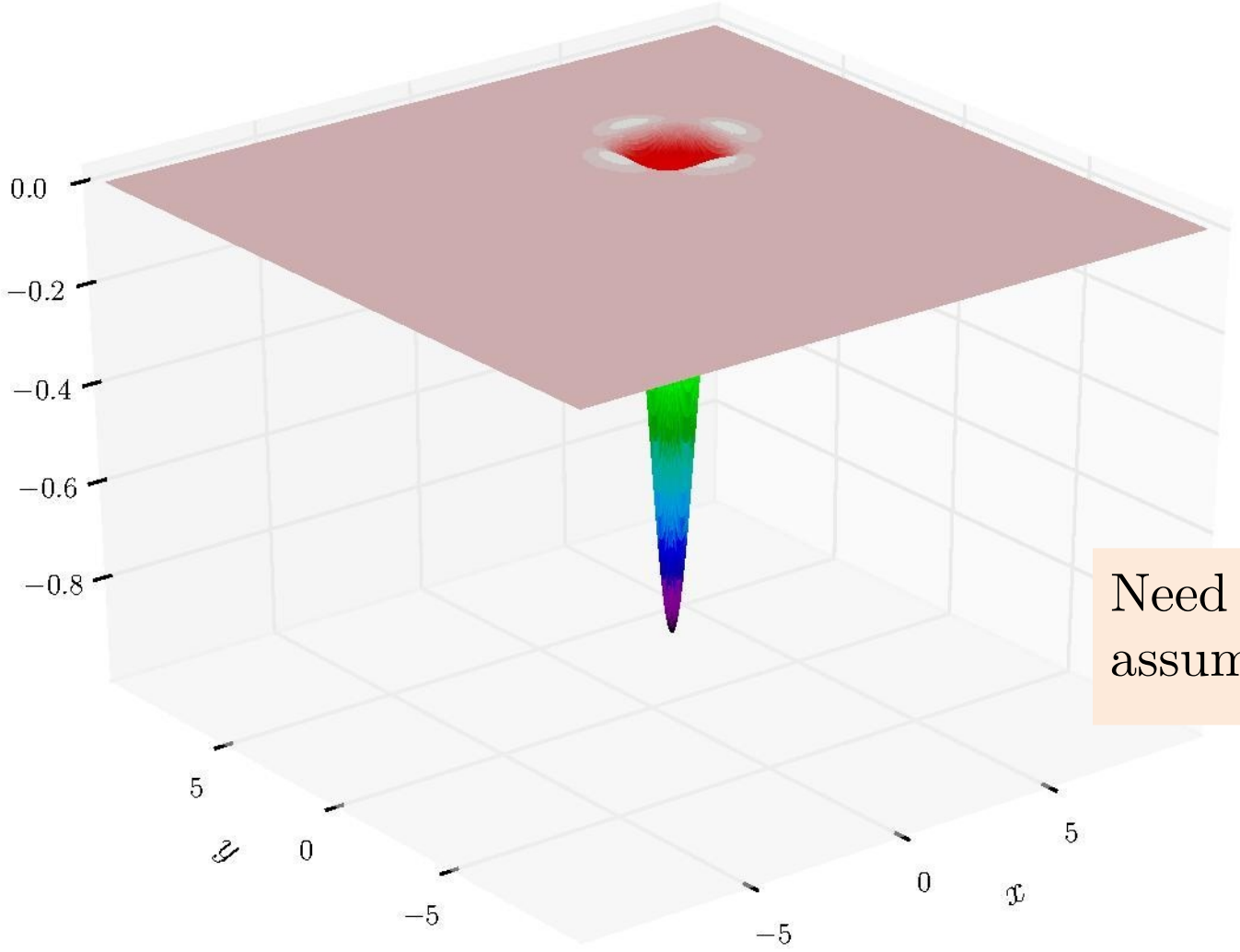
Specialize

Convex and smooth training problems

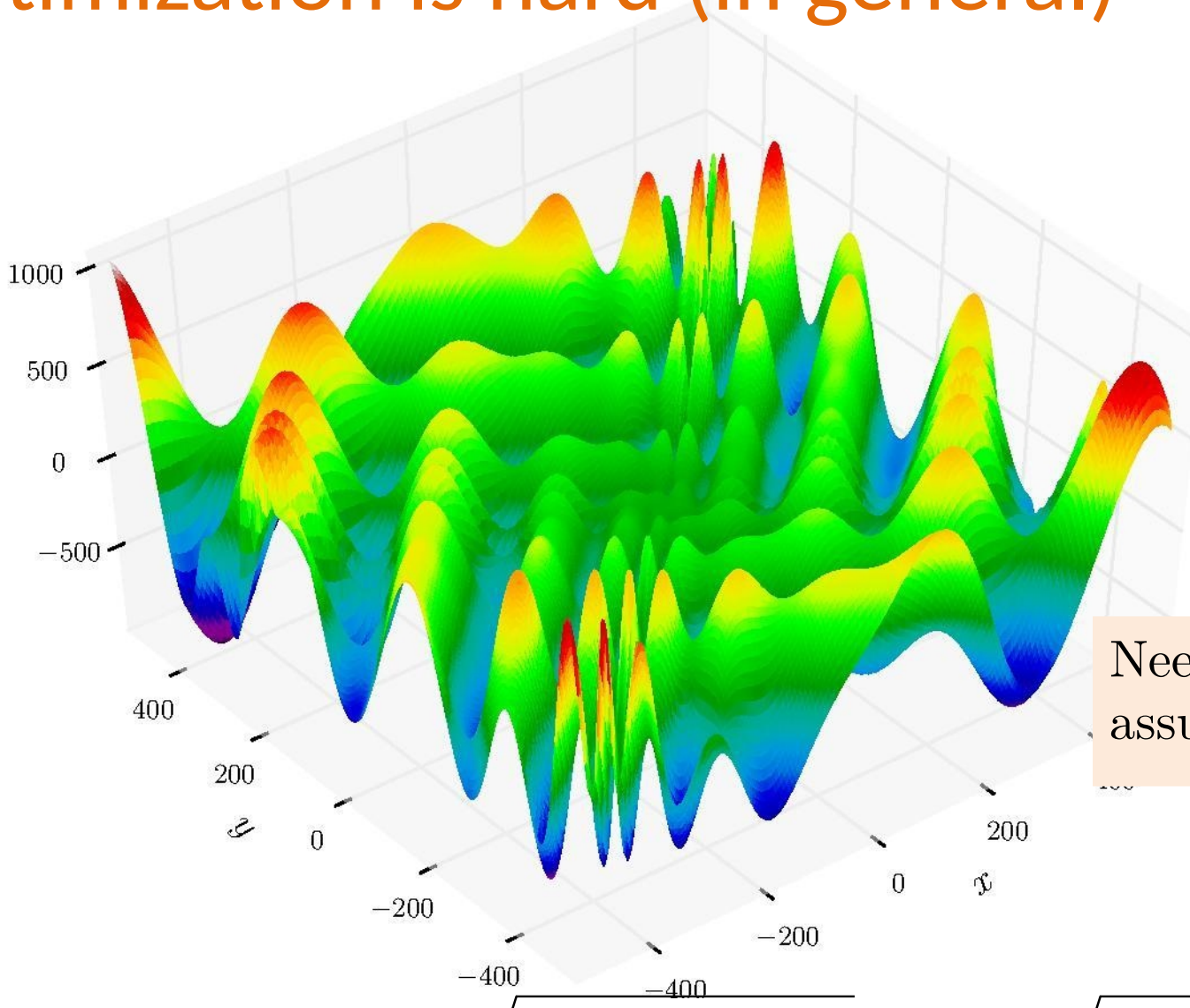
Optimization is hard (in general)



Need assumptions!

$$f(x, y) = -\cos(x)\cos(y)\exp\left(-(x-\pi)^2 - (y-\pi)^2\right)$$

Optimization is hard (in general)



Need assumptions!

$$f(x,y) = -(y+47)\sin\sqrt{\left|\frac{x}{2}+(y+47)\right|} - x\sin\sqrt{\left|\frac{x}{2}-(y+47)\right|}$$

Main assumption

Nice property

$$\text{If } \nabla f(w^*) = 0 \quad \text{then} \quad f(w^*) \leq f(w), \quad \forall w \in \mathbb{R}^d$$

All stationary points are global minima

Lemma: Convexity => Nice property

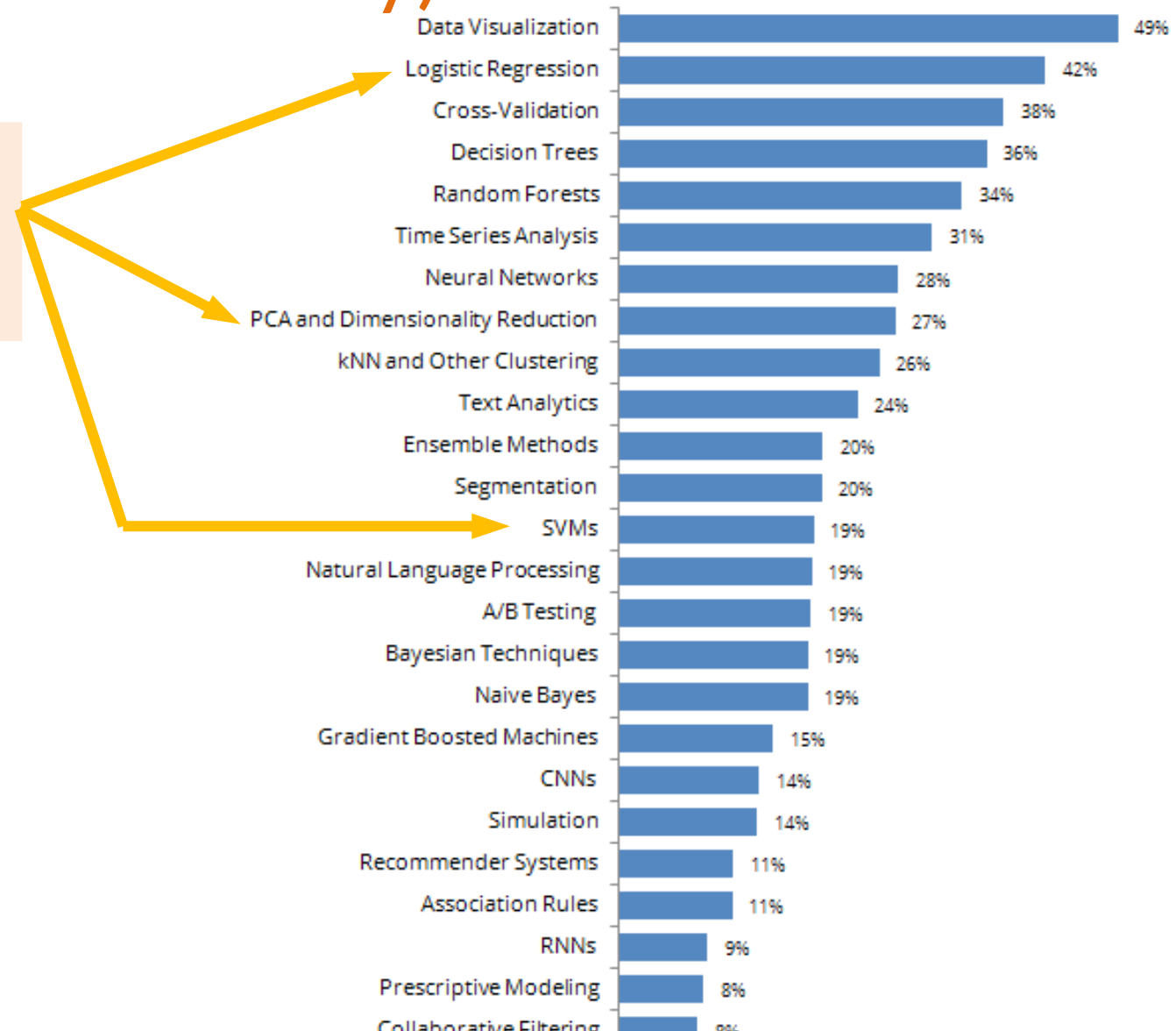
$$\text{If } \; f(w) \geq f(y) + \langle \nabla f(y), w - y \rangle, \quad \forall w, y \in \mathbb{R}^d$$

then nice property holds

PROOF: Choose $y = w^*$

Data science methods most used (Kaggle 2017 survey)

Convex Optimization problems



Part III: Stochastic Gradient Descent

The Training Problem

Solving the *training problem*:

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} f_i(w)$$

Problem with Gradient Descent:
Each iteration requires computing a gradient $\nabla f_i(w)$ for each data point. One gradient for each cat on the internet!

Gradient Descent Algorithm

Set $w^0 = 0$, choose $\alpha > 0$.
for $t = 0, 1, 2, \ldots, T$
$$w^{t+1} = w^t - \frac{\alpha}{n} \sum_{i=1}^{n} \nabla f_i(w^t)$$
Output w^T

Stochastic Gradient Descent

Is it possible to design a method that uses only the gradient of a **single** data function $f_i(w)$ at each iteration?

Stochastic Gradient Descent

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Unbiased Estimate

Let j be a random index sampled from $\{1, \ldots, n\}$ selected uniformly at random. Then

$$\mathbb{E}_j[\nabla f_j(w)] \;=\; \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(w) \;=\; \nabla f(w)$$

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Use $\nabla f_j(w) \approx \nabla f(w)$

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Use $\nabla f_j(w) \approx \nabla f(w)$

EXE: Let $\sum_{i=1}^{n} p_i = 1$ and $j \sim p_j$. Show $\mathbb{E}[\nabla f_j(w)/(np_j)] = \nabla f(w)$

Stochastic Gradient Descent

SGD 0.0 Constant stepsize

Set $w^0 = 0$, choose $\alpha > 0$

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

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

$w^{t+1} = w^t - \alpha \nabla f_j(w^t)$

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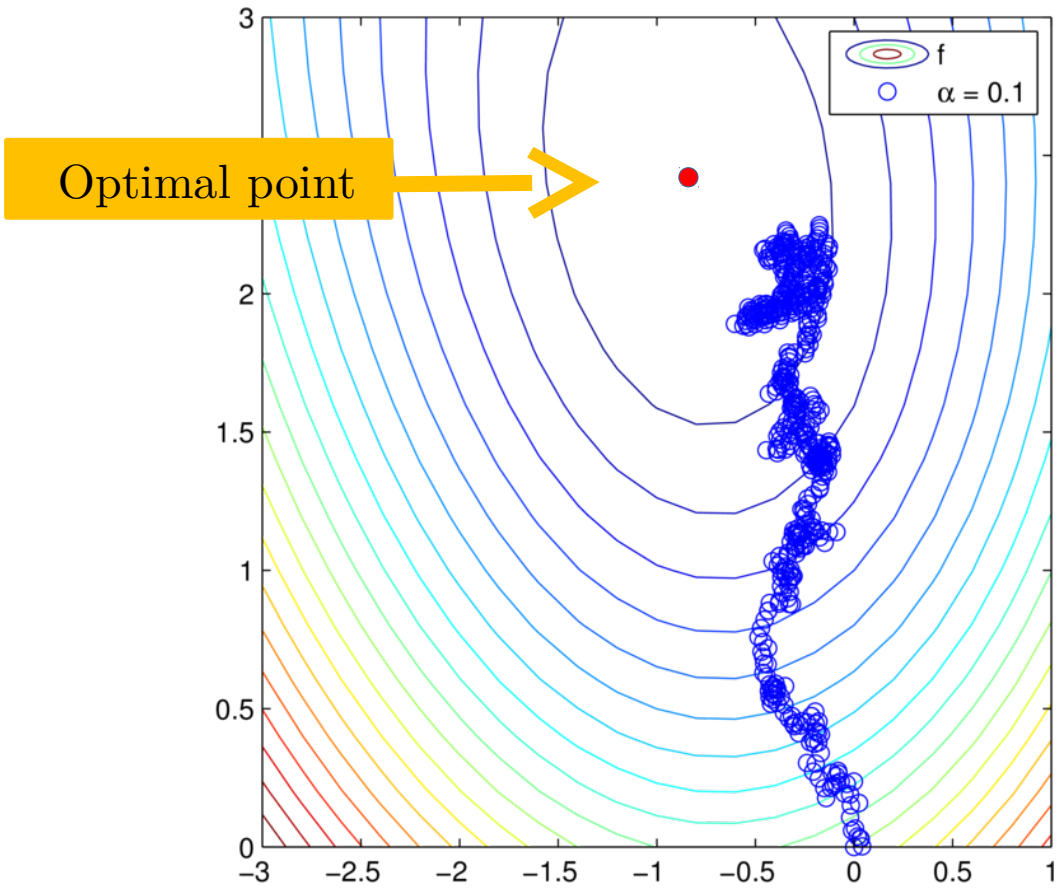
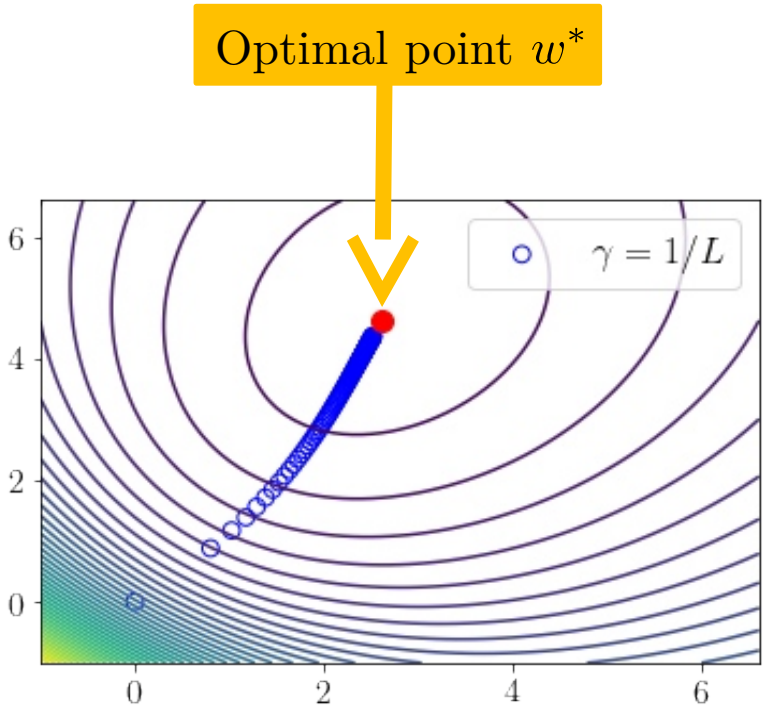
Stochastic Gradient Descent



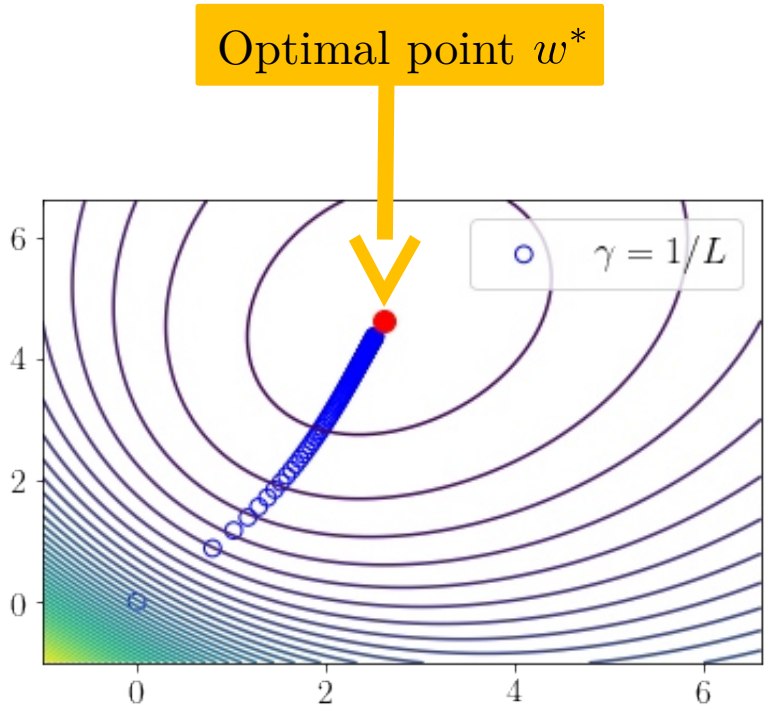
GD vs Stochastic Gradient Descent



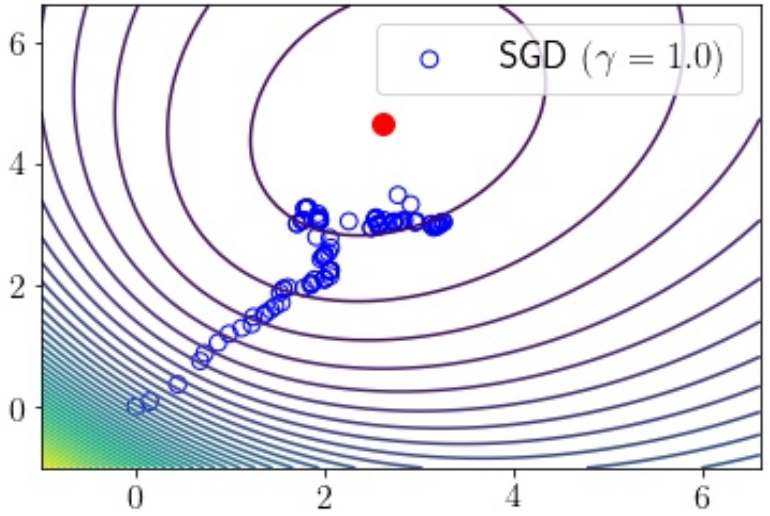
Gradient Descent

Need Assumptions

GD vs Stochastic Gradient Descent



Gradient Descent



Stochastic Gradient Descent

Why does this happen?

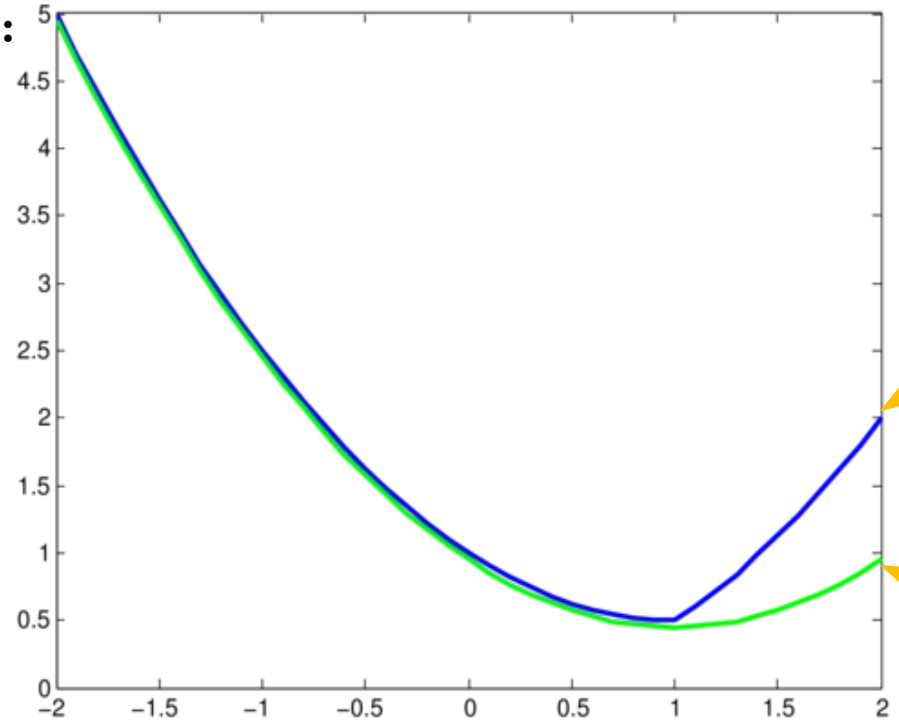
Need Assumptions

Assumption: Strong convexity

We say $f : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ is μ–strongly convex if

$$f(w) \geq f(y) + \langle \nabla f(y), w - y \rangle + \frac{\mu}{2}||w - y||^2, \quad \forall w, y \in \mathbb{R}^n$$

EXE:



Hinge loss + L2

$$\max\{0, 1 - w\} + \frac{1}{2}||w||_2^2$$

Quadratic lower bound

Assumption: Strong convexity

$$f(w) := \frac{1}{n}\sum_{i=1}^{n} \underbrace{\ell\left(h_w(x^i), y^i\right)}_{\|} + \underbrace{\lambda R(w)}_{\|}$$

$$\text{strongly convex} \quad = \quad \text{convex} \quad + \quad \frac{1}{2}\|w\|^2$$

Example: SVM with soft margin

$$\min_{w \in \mathbf{R}^d} \frac{1}{n}\sum_{i=1}^{n} \max\{0, 1 - y^i \langle w, x^i \rangle\} + \frac{\lambda}{2}||w||_2^2$$

Not an Example: Neural networks, dictionary learning, And more

Assumption: Smoothness

We say $f : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ is smooth if

$$||\nabla f(x) - \nabla f(y)|| \leq L||x - y||, \quad \forall x, y \in \mathbb{R}^n$$

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If a twice differentiable $f : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ is L–smooth then

1) $$d^\top \nabla^2 f(x) d \leq L \cdot ||d||_2^2, \quad \forall x, d \in \mathbb{R}^n$$

2) $$f(x) \leq f(y) + \langle \nabla f(y), x - y \rangle + \frac{L}{2}||x - y||^2, \quad \forall x, y \in \mathbb{R}^n$$

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EXE: Using that $\sigma_{\max}(X)^2 ||d||_2^2 \geq ||X^\top d||_2^2$

Show that $\frac{1}{2}||X^\top w - b||_2^2$ is $\sigma_{\max}(X)^2$–smooth

Smoothness: Examples

Convex quadratics: $x \mapsto x^\top A x + b^\top x + c$

Logistic: $x \mapsto \log\left(1 + e^{-y\langle a, x\rangle}\right)$

Trigonometric: $x \mapsto \cos(x), \sin(x)$

Proof is an exercise!

Important consequences of Smoothness

If $f : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ is L–smooth then

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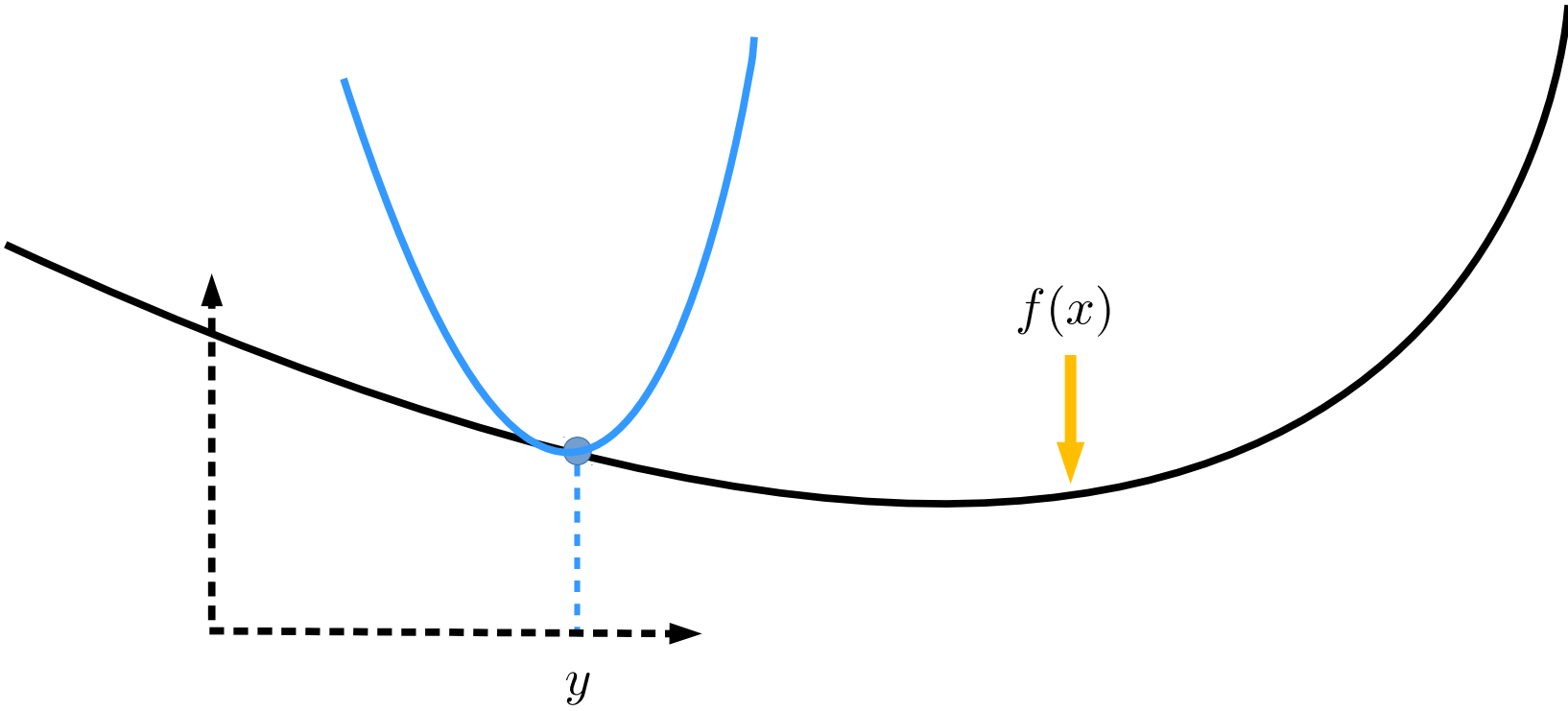
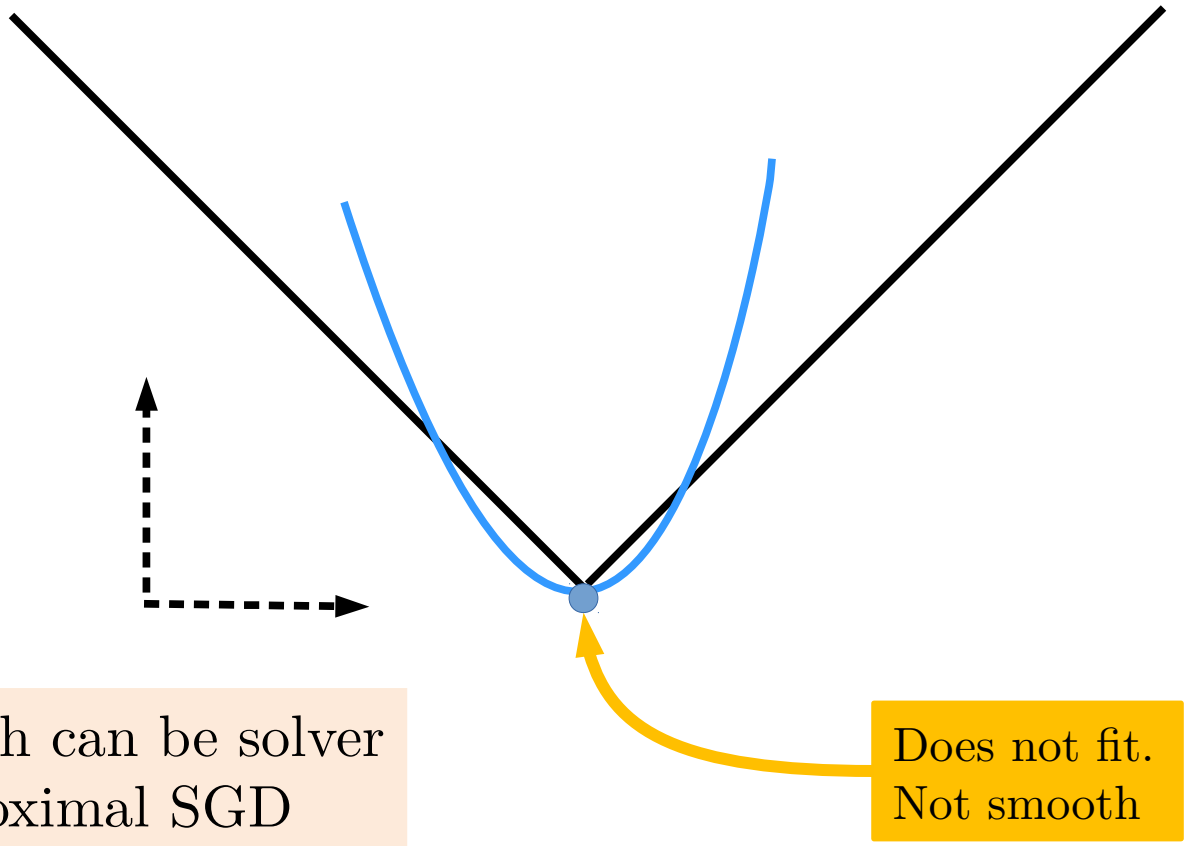


Smoothness: Convex counter-example

$$f(w) = ||w||_1 = \sum_{i=1}^{n} |w_i|$$



Non-smooth can be solver with proximal SGD

Does not fit. Not smooth

Assumptions for Convergence

Strongly quasi-convexity

$$f(w^*) \geq f(w) + \langle \nabla f(w), w^* - w \rangle + \frac{\mu}{2}||w^* - w||_2^2, \quad \forall w$$

Each f_i is convex and L_i smooth

$$f_i(y) \leq f_i(w) + \langle \nabla f_i(w), y - w \rangle + \frac{L_i}{2}||y - w||_2^2, \quad \forall w$$

$$L_{\max} := \max_{i=1,\ldots,n} L_i$$

Definition: Gradient Noise

$$\sigma^2 \quad := \quad \mathbb{E}_j[||\nabla f_j(w^*)||_2^2]$$

Assumptions for Convergence

EXE: Calculate the L_i's and L_{max} for

1. $f(w) = \frac{1}{2n}||X^\top w - y||_2^2 + \frac{\lambda}{2}||w||_2^2$

HINT: A twice differentiable f_i is L_i-smooth if and only if

$$\nabla^2 f_i(w) \preceq L_i \, I \quad \Leftrightarrow \quad v^\top \nabla^2 f_i(w) v \leq L_i \|v\|^2, \forall v$$

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$$L_{\max} = \max_{i=1,\ldots,n}(||x_i||_2^2 + \lambda) = \max_{i=1,\ldots,n} ||x_i||_2^2 + \lambda$$

Assumptions for Convergence

EXE: Calculate the L_i's and L_{max} for

2. $$f(w) = \frac{1}{n}\sum_{i=1}^{n} \ln(1 + e^{-y_i \langle w, a_i \rangle}) + \frac{\lambda}{2}||w||_2^2$$

Assumptions for Convergence

EXE: Calculate the L_i's and L_{max} for

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Assumptions for Convergence

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$$2. \quad f_i(w) = \ln(1 + e^{-y_i \langle w, a_i \rangle}) + \frac{\lambda}{2}||w||_2^2,$$

$$\nabla f_i(w) = \frac{-y_i a_i e^{-y_i \langle w, a_i \rangle}}{1 + e^{-y_i \langle w, a_i \rangle}} + \lambda w$$

$$\nabla^2 f_i(w) = a_i a_i^\top \left(\frac{(1 + e^{-y_i \langle w, a_i \rangle}) e^{-y_i \langle w, a_i \rangle}}{(1 + e^{-y_i \langle w, a_i \rangle})^2} - \frac{e^{-2y_i \langle w, a_i \rangle}}{(1 + e^{-y_i \langle w, a_i \rangle})^2} \right) + \lambda I$$

$$= a_i a_i^\top \frac{e^{-y_i \langle w, a_i \rangle}}{(1 + e^{-y_i \langle w, a_i \rangle})^2} + \lambda I \quad \preceq \quad \left(\frac{||a_i||_2^2}{4} + \lambda \right) I = L_i \, I$$

Complexity / Convergence

Theorem

If f is μ-strongly convex f_i is L_i–smooth and $0 < \alpha \leq \frac{1}{2L_{\max}}$ then the iterates of the SGD satisfy

$$\mathbb{E}\left[||w^t - w^*||_2^2\right] \leq (1 - \alpha\mu)^t ||w^0 - w^*||_2^2 + \frac{2\alpha}{\mu}\sigma^2$$

Shows that $\alpha \approx \frac{1}{\lambda}$

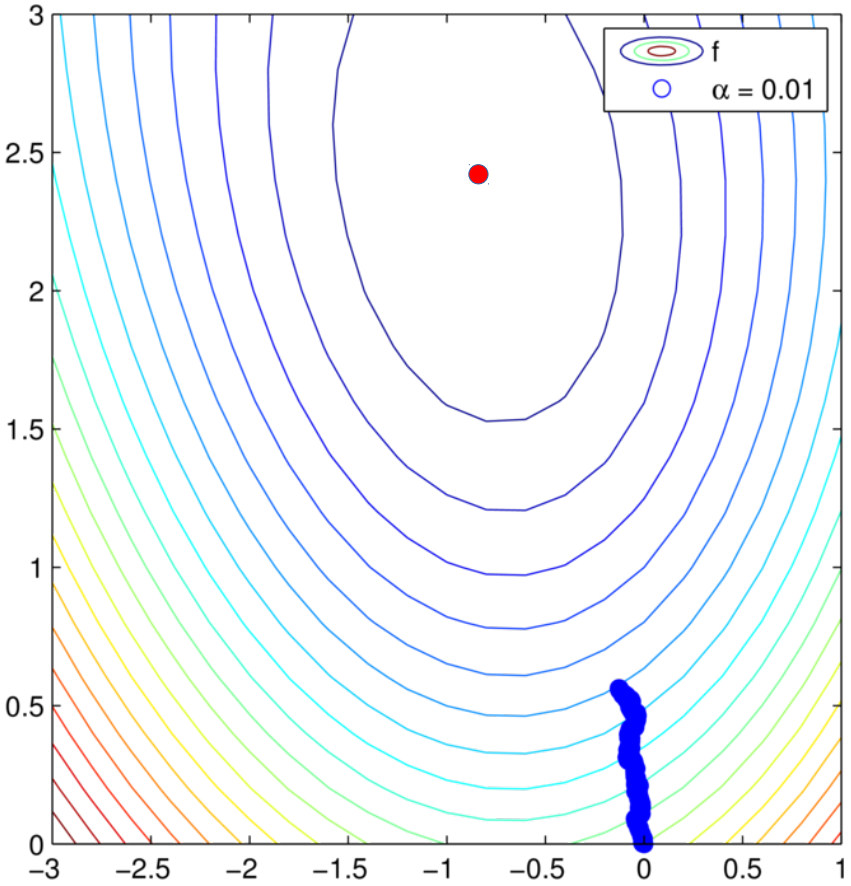
Shows that $\alpha \approx 0$

RMG, N. Loizou, X. Qian, A. Sailanbayev, E. Shulgin, P. Richtarik, ICML 2019, arXiv:1901.09401

SGD: General Analysis and Improved Rates.

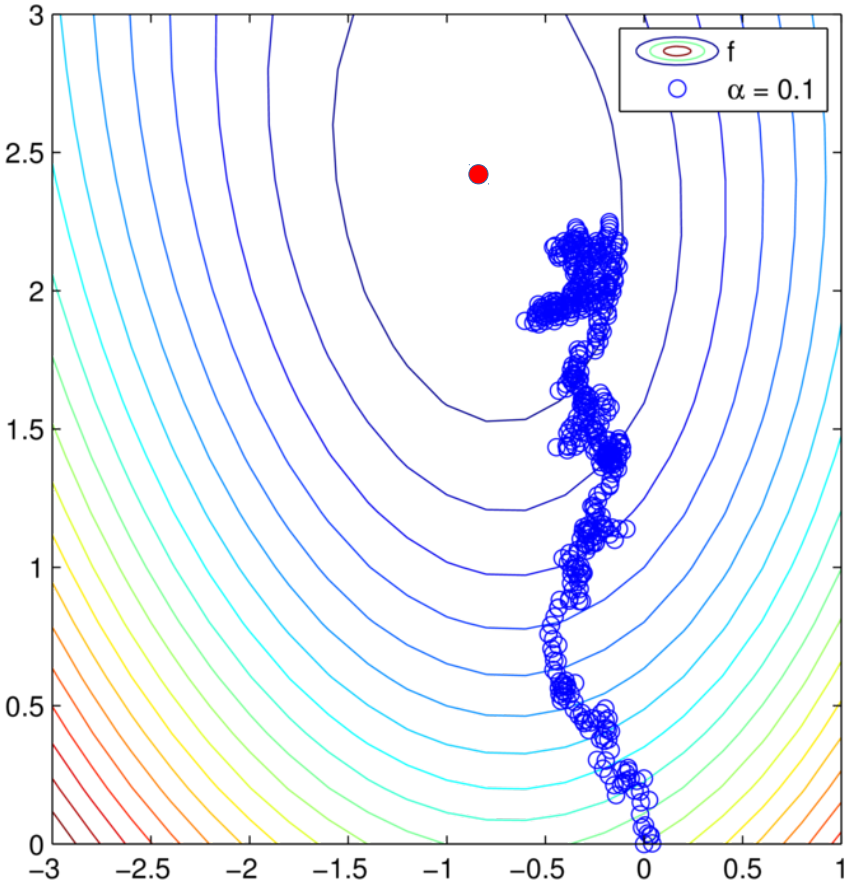
Stochastic Gradient Descent

α =0.01



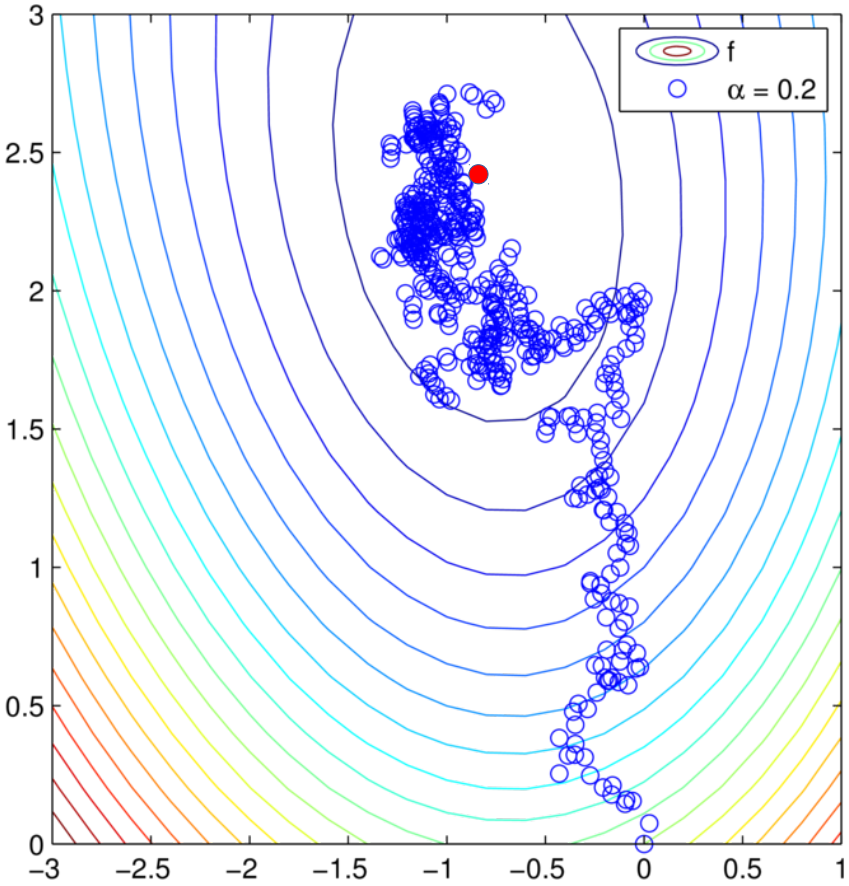
Stochastic Gradient Descent

α =0.1



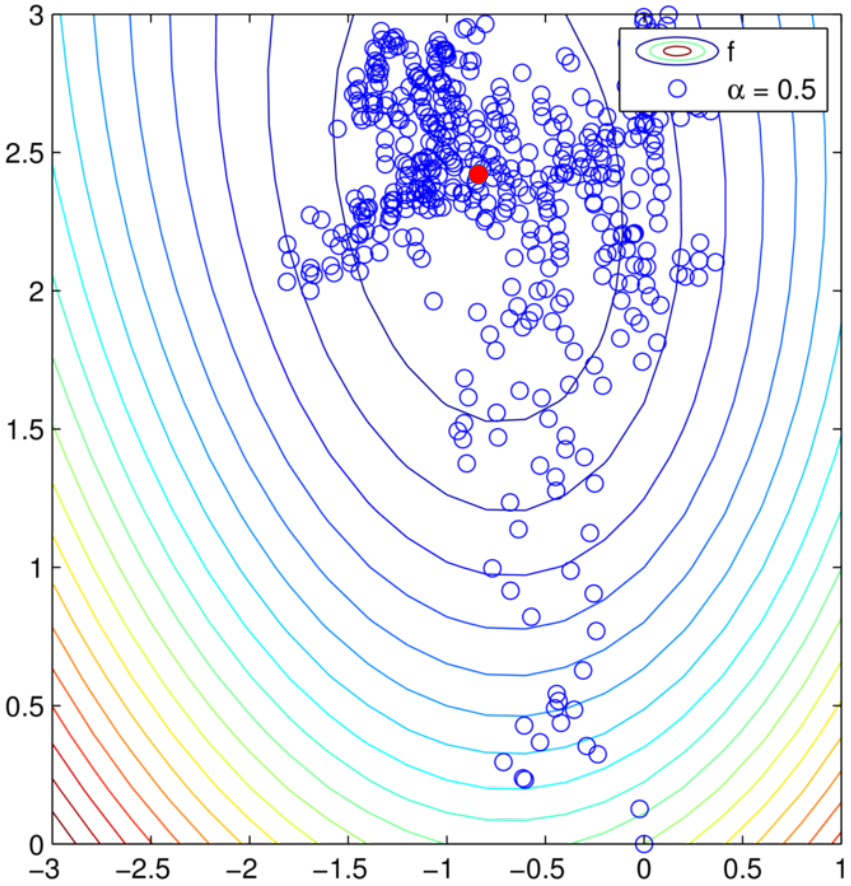
Stochastic Gradient Descent

α =0.2



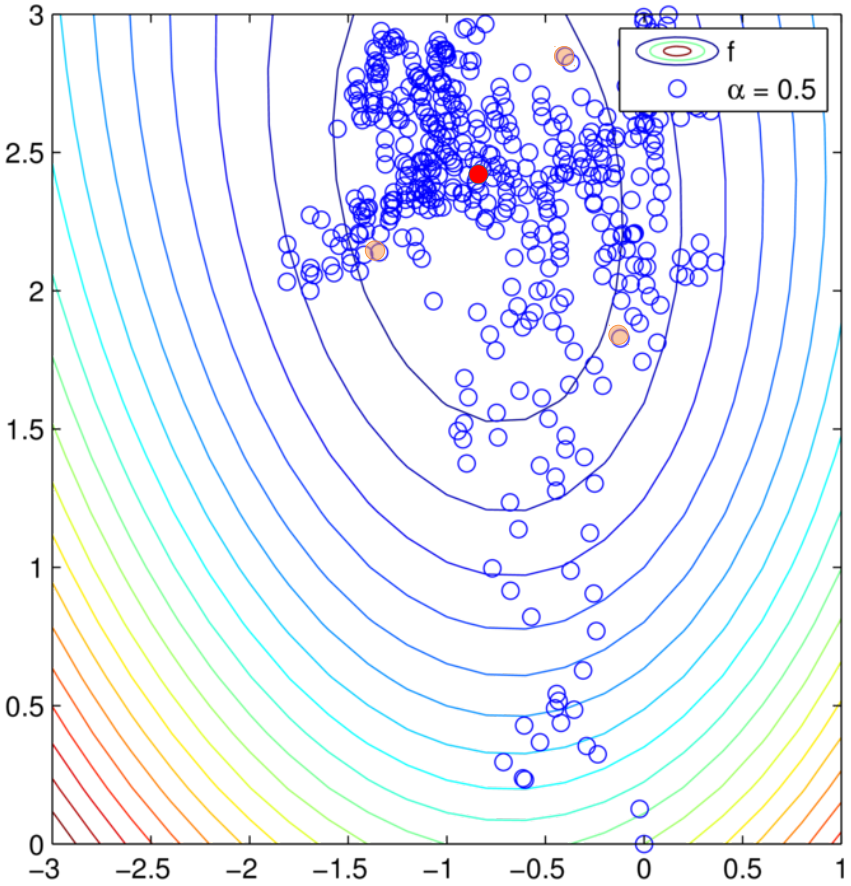
Stochastic Gradient Descent

α =0.5



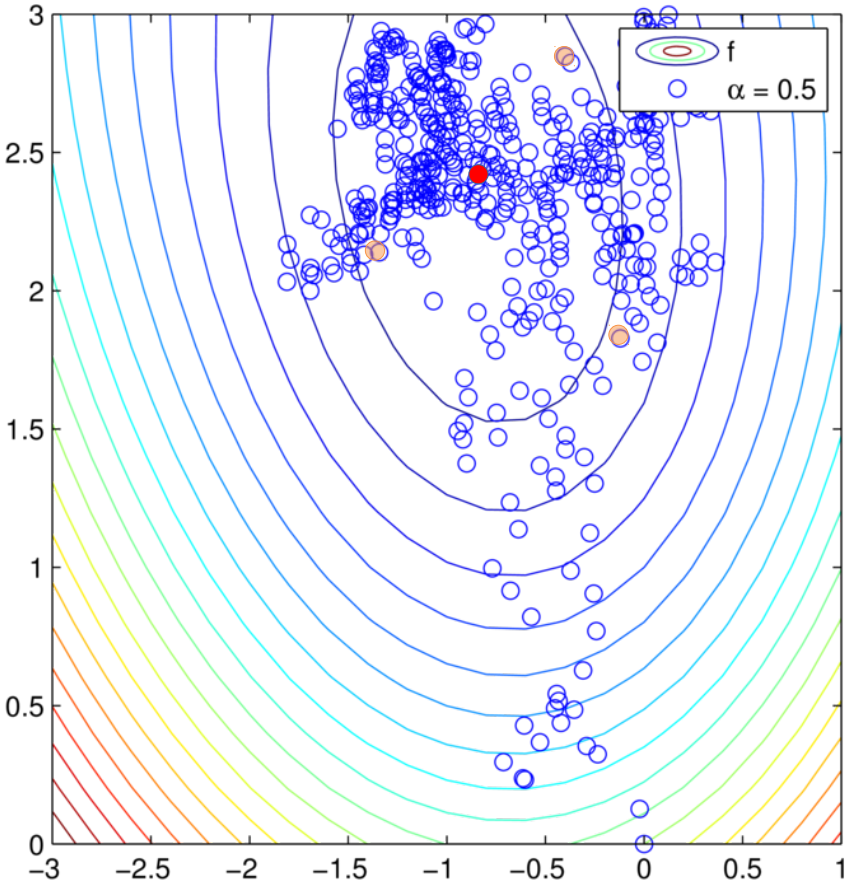
Stochastic Gradient Descent

α =0.5



Stochastic Gradient Descent

α =0.5

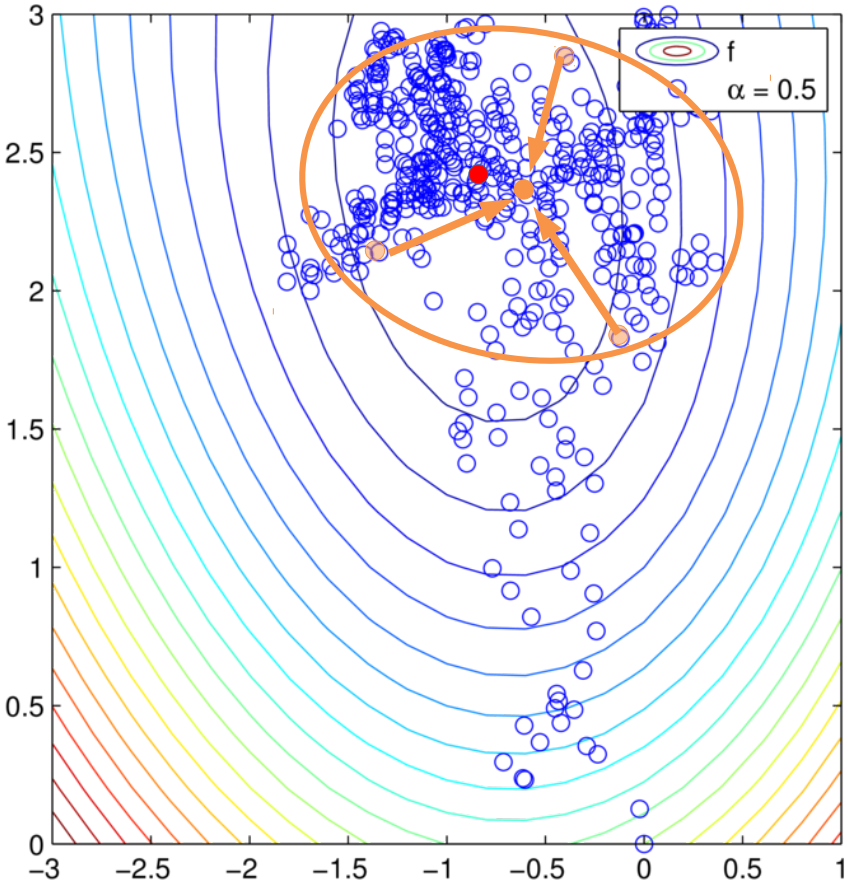


1) Start with big steps and end with smaller steps

2) Try averaging the points

Stochastic Gradient Descent

α =0.5



1) Start with big steps and end with smaller steps

2) Try averaging the points

SGD shrinking stepsize

SGD Shrinking stepsize

Set $w^0 = 0$

Choose $\alpha_t > 0$, $\alpha_t \to 0$, $\sum_{t=0}^{\infty} \alpha_t = \infty$

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

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

$w^{t+1} = w^t - \alpha_t \nabla f_j(w^t)$

Output w^T

Shrinking Stepsize

SGD shrinking stepsize

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$w^{t+1} = w^t - \alpha_t \nabla f_j(w^t)$

Output w^T

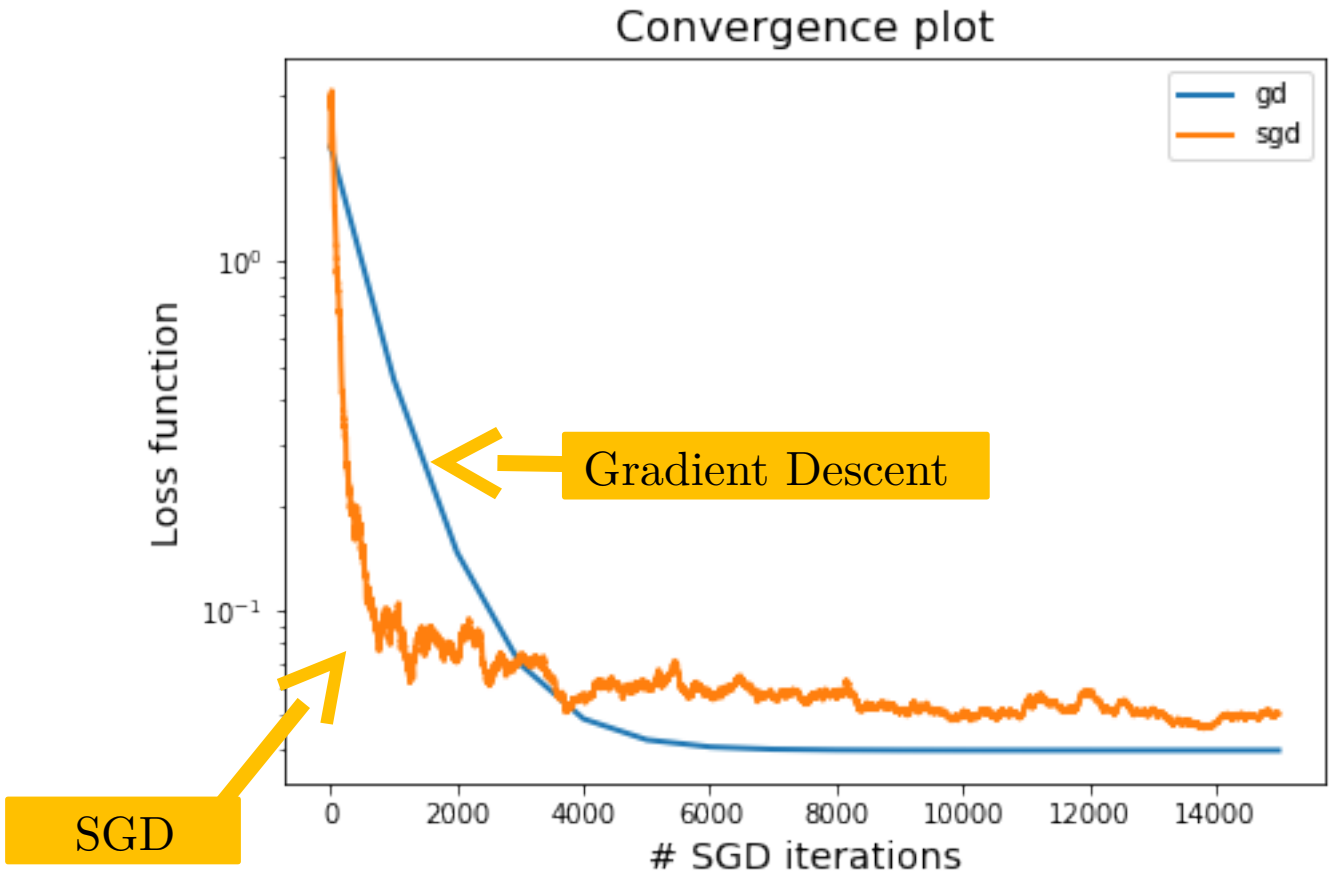
Shrinking Stepsize

How should we sample j ?

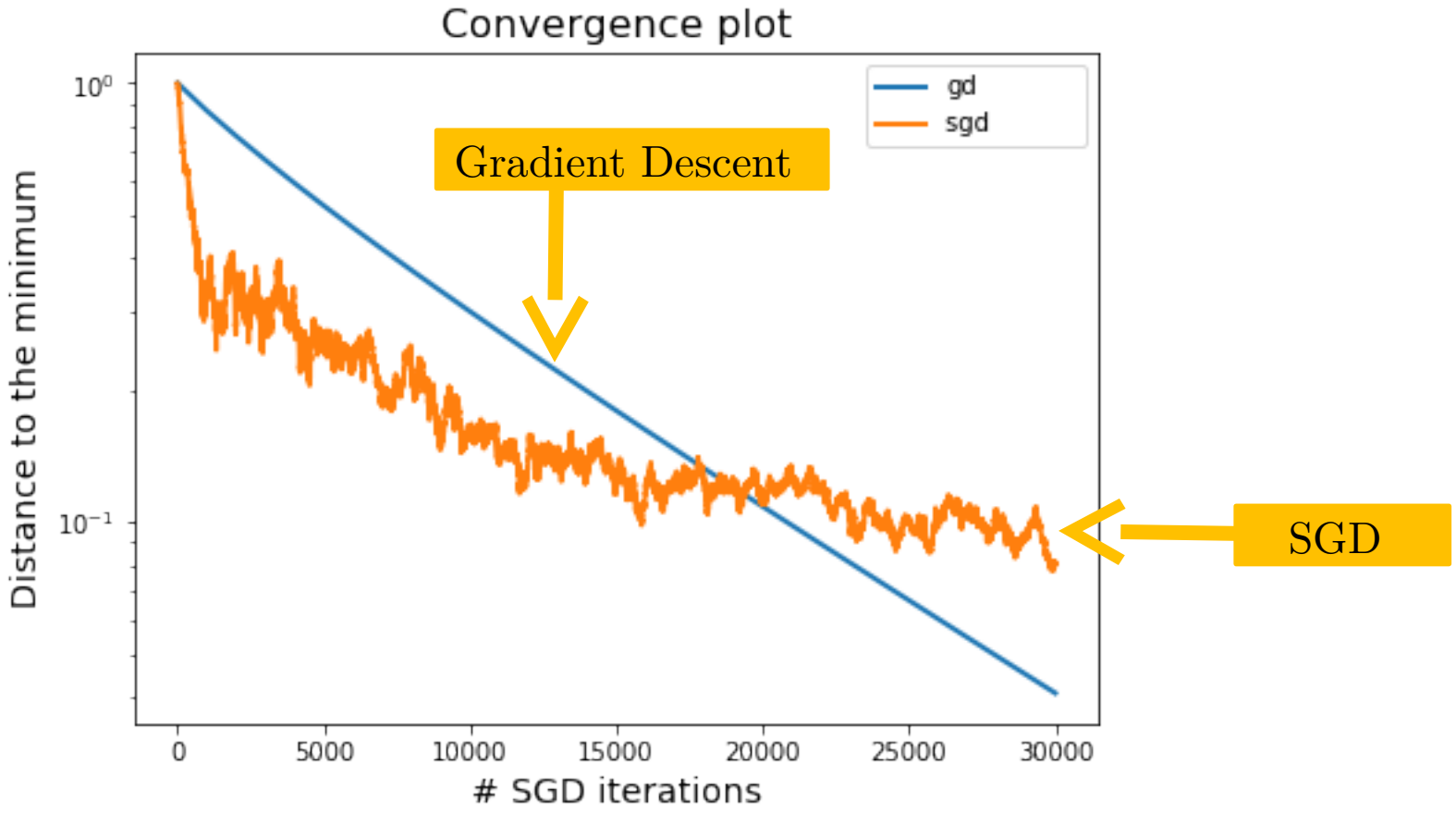
How fast $\alpha_t \to 0$?

Does this converge?

SGD with shrinking stepsize
Compared with Gradient Descent



SGD with shrinking stepsize Compared with Gradient Descent



Complexity / Convergence

Theorem for switching to shrinking stepsizes

Let f be μ-strongly convex and f_i is L_i–smooth

Let $\mathcal{K} := L_{\max}/\mu$ and let

$$\alpha^t = \begin{cases} \frac{1}{2L_{\max}} & \text{for} \quad t \leq 4\lceil \mathcal{K} \rceil \\ \frac{2t+1}{(t+1)^2\mu} & \text{for} \quad t > 4\lceil \mathcal{K} \rceil. \end{cases}$$

If $t \geq 4\lceil \mathcal{K} \rceil$, then the SGD iterates converge

$$\mathbb{E}\|w^t - w^*\|^2 \leq \frac{\sigma^2}{\mu^2}\frac{8}{t} + \frac{16}{e^2}\frac{\lceil \mathcal{K} \rceil^2}{t^2}\|w^0 - w^*\|^2$$

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$\alpha^t = O(1/(t+1))$

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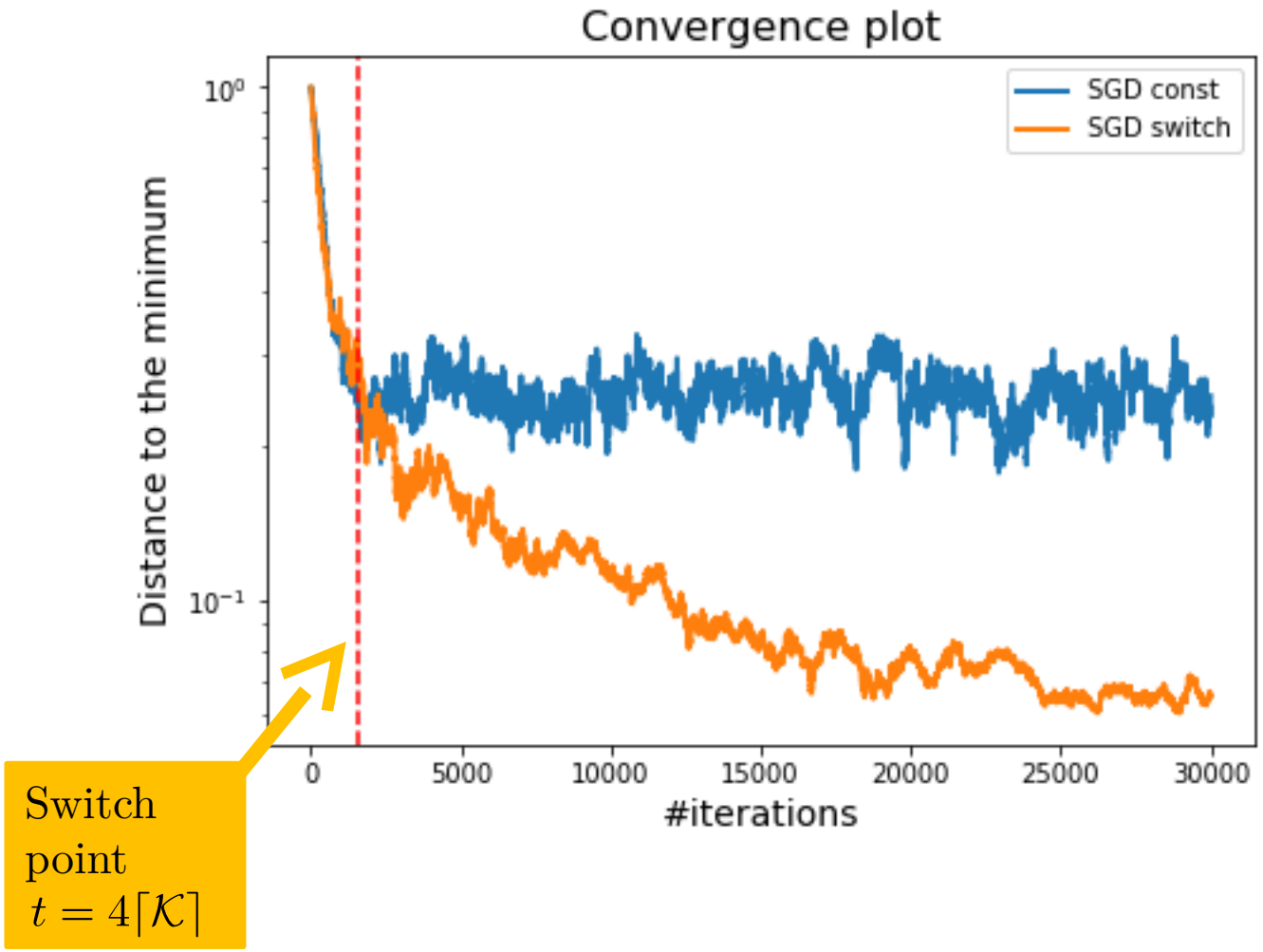
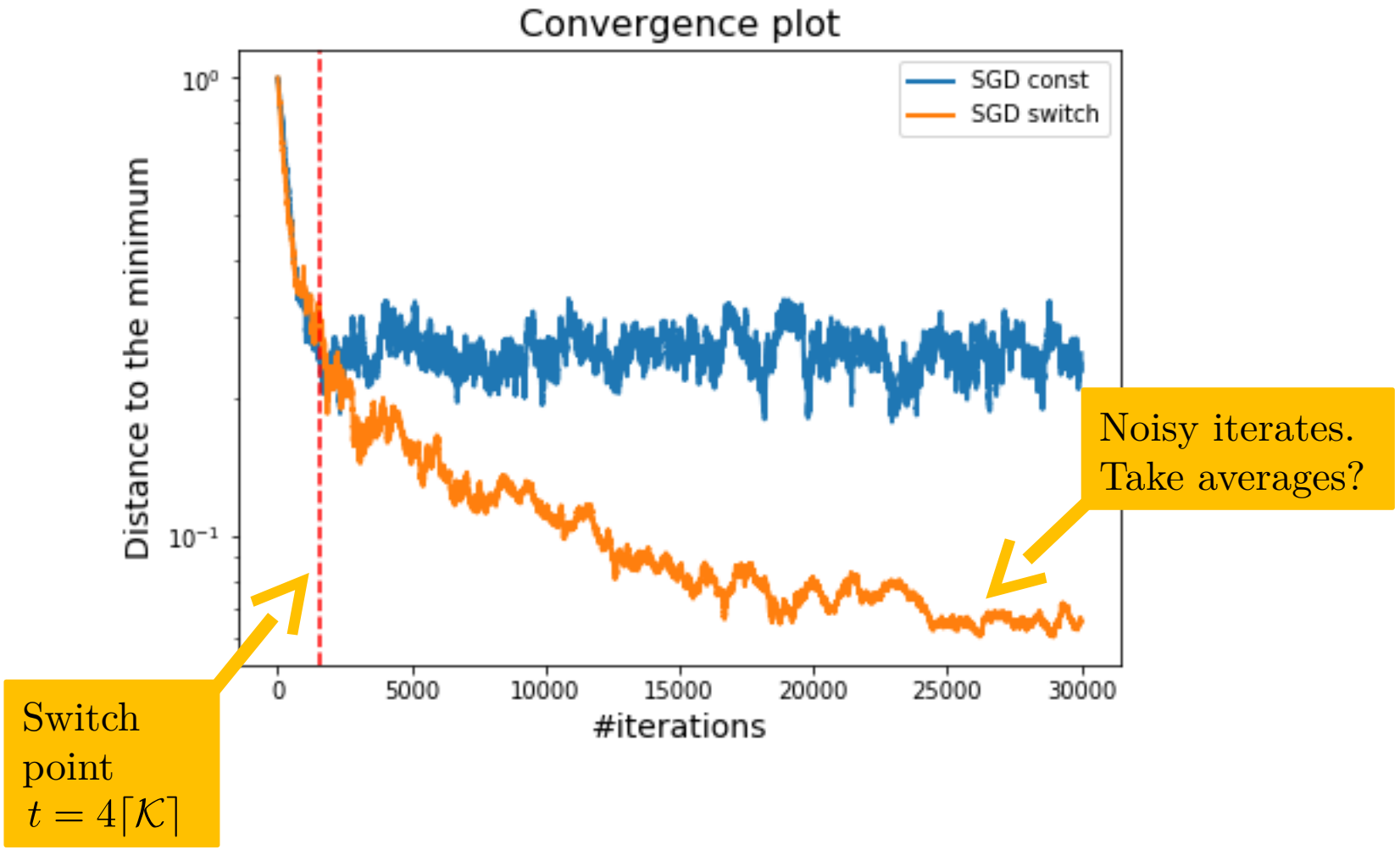
In practice often $\alpha^t = C/\sqrt{t+1}$ where C is tuned

Stochastic Gradient Descent with switch to decreasing stepsizes



Stochastic Gradient Descent with switch to decreasing stepsizes



SGD with (late start) averaging

SGD with late averaging

Set $w^0 = 0$

Choose $\alpha_t > 0$, $\alpha_t \to 0$, $\sum_{t=0}^{\infty} \alpha_t = \infty$

Choose averaging start $s_0 \in \mathbb{N}$

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

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

$w^{t+1} = w^t - \alpha_t \nabla f_j(w^t)$

if $t > s_0$

$\overline{w} = \frac{1}{t - s_0} \sum_{i=s_0}^{t} w^t$

else: $\overline{w} = w$

Output $\overline{w}$

B. T. Polyak and A. B. Juditsky, SIAM Journal on Control and Optimization (1992)
Acceleration of stochastic approximation by averaging

SGD with (late start) averaging

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if $t > s_0$

$\overline{w} = \frac{1}{t - s_0} \sum_{i=s_0}^{t} w^t$

else: $\overline{w} = w$

Output $\overline{w}$

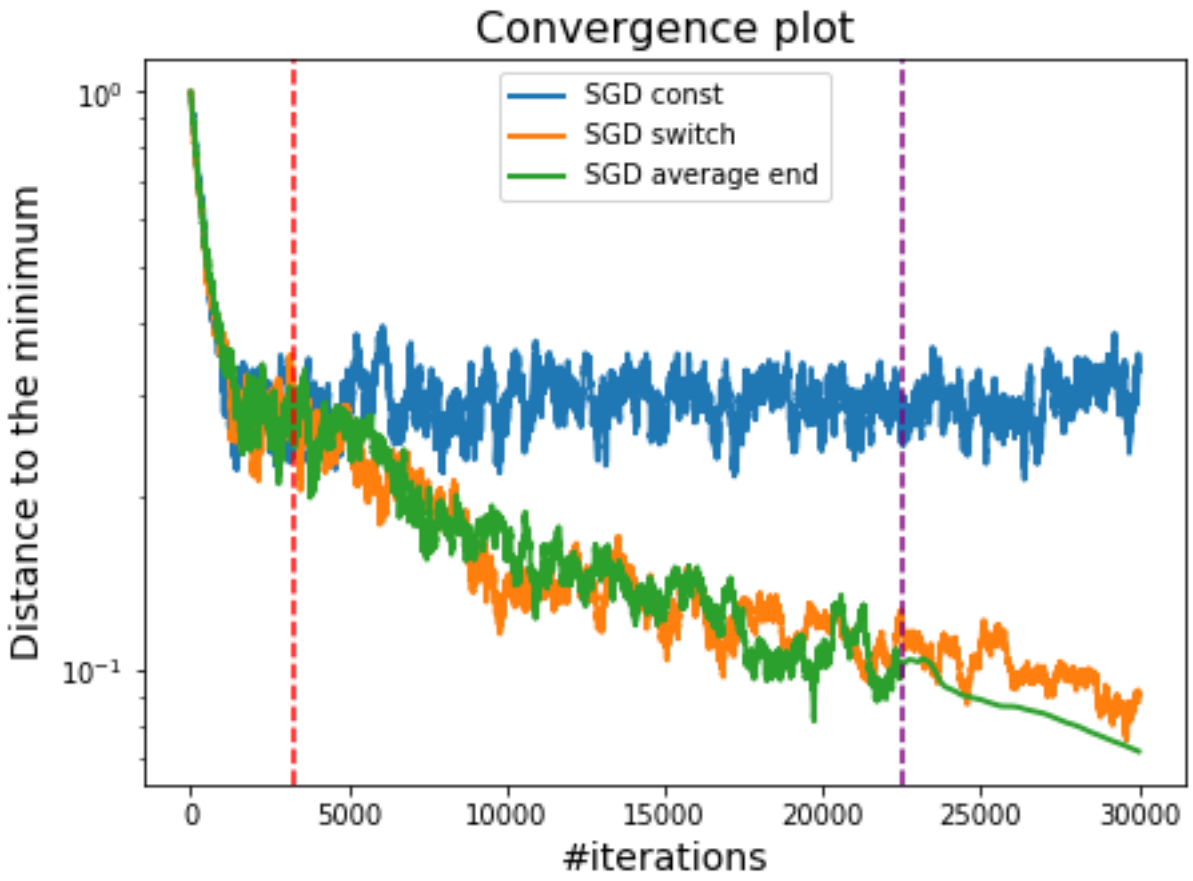
This is not efficient. How to make this efficient?

B. T. Polyak and A. B. Juditsky, SIAM Journal on Control and Optimization (1992)

Acceleration of stochastic approximation by averaging

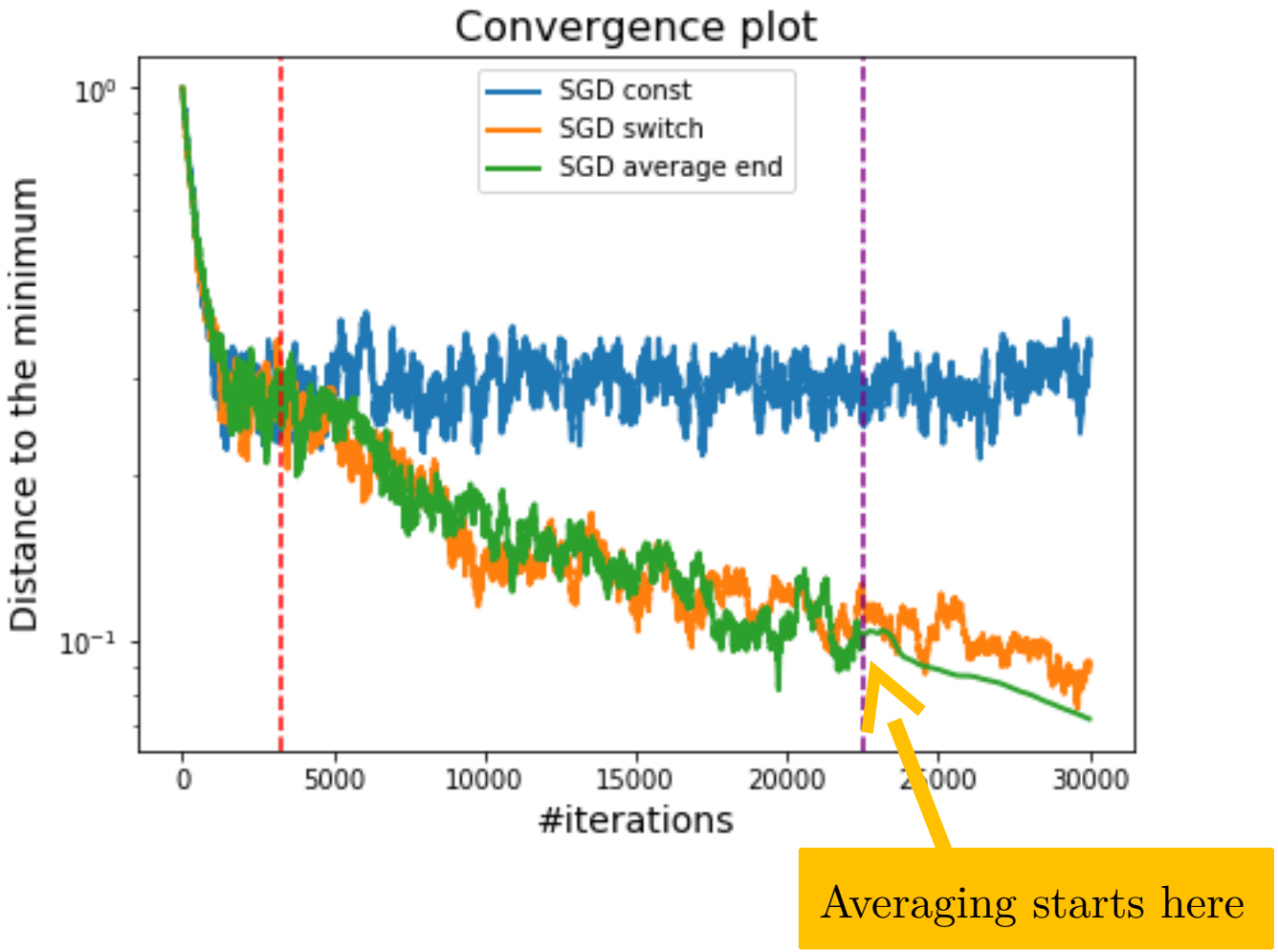
Stochastic Gradient Descent

Averaging the last few iterates



Stochastic Gradient Descent

Averaging the last few iterates



Part III.2: Stochastic Gradient Descent for Sparse Data

Lazy SGD updates for Sparse Data

L2 regularizor + linear hypothesis

Finite Sum Training Problem

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \ell\left(\langle w, x^i \rangle, y^i\right) + \frac{\lambda}{2}||w||_2^2$$

Assume each data point x^i is s-sparse, how many operations does each SGD step cost?

Sparse Examples: encoding of categorical variables (hot one encoding), word2vec, recommendation systems ...etc

Lazy SGD updates for Sparse Data

L2 regularizor + linear hypothesis

Finite Sum Training Problem

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \ell\left(\langle w, x^i \rangle, y^i\right) + \frac{\lambda}{2}||w||_2^2$$

Assume each data point x^i is s-sparse, how many operations does each SGD step cost?

$$\begin{aligned} w^{t+1} &= w^t - \alpha_t \left(\ell'(\langle w^t, x^i \rangle, y^i) x^i + \lambda w^t\right) \\ &= (1 - \lambda \alpha_t) w^t - \alpha_t \ell'(\langle w^t, x^i \rangle, y^i) x^i \end{aligned}$$

Sparse Examples: encoding of categorical variables (hot one encoding), word2vec, recommendation systems ...etc

Lazy SGD updates for Sparse Data

L2 regularizor + linear hypothesis

Finite Sum Training Problem

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \ell\left(\langle w, x^i \rangle, y^i\right) + \frac{\lambda}{2}||w||_2^2$$

Assume each data point x^i is s-sparse, how many operations does each SGD step cost?

$$\begin{aligned} w^{t+1} &= w^t - \alpha_t \left(\ell'(\langle w^t, x^i \rangle, y^i) x^i + \lambda w^t\right) \\ &= \underbrace{(1 - \lambda\alpha_t) w^t}_{\text{Rescaling } O(d)} \underbrace{- \alpha_t \ell'(\langle w^t, x^i \rangle, y^i) x^i}_{\text{Addition sparse vector } O(s)} \end{aligned}$$

$+ \quad = \quad O(d)$

Sparse Examples: encoding of categorical variables (hot one encoding), word2vec, recommendation systems ...etc

Lazy SGD updates for Sparse Data

SGD step

$$w^{t+1} = (1 - \lambda\alpha_t)w^t - \alpha_t \ell'(\langle w^t, x^i \rangle, y^i)x^i$$

EXE: re-write the iterates using $w^t = \beta_t z^t$ where $\beta_t \in \mathbb{R},\ z^t \in \mathbb{R}^d$

Can you update β_t and z^t so that each iteration is $O(s)$?

Lazy SGD updates for Sparse Data

SGD step

$$w^{t+1} = (1 - \lambda\alpha_t)w^t - \alpha_t \ell'(\langle w^t, x^i \rangle, y^i)x^i$$

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Can you update β_t and z^t so that each iteration is $O(s)$?

$$\begin{aligned}
\beta_{t+1} z^{t+1} &= (1 - \lambda\alpha_t)\beta_t z^t - \alpha_t \ell'(\beta_t \langle z^t, x^i \rangle, y^i)x^i \\
&= (1 - \lambda\alpha_t)\beta_t \left(z^t - \frac{\alpha_t \ell'(\beta_t \langle z^t, x^i \rangle, y^i)}{(1 - \lambda\alpha_t)\beta_t} x^i \right)
\end{aligned}$$

Lazy SGD updates for Sparse Data

SGD step

$$w^{t+1} = (1 - \lambda\alpha_t)w^t - \alpha_t \ell'(\langle w^t, x^i \rangle, y^i) x^i$$

EXE: re-write the iterates using $w^t = \beta_t z^t$ where $\beta_t \in \mathbb{R}$, $z^t \in \mathbb{R}^d$

Can you update β_t and z^t so that each iteration is $O(s)$?

$$\begin{aligned}
\beta_{t+1} z^{t+1} &= (1 - \lambda\alpha_t)\beta_t z^t - \alpha_t \ell'(\beta_t \langle z^t, x^i \rangle, y^i) x^i \\
&= \underbrace{(1 - \lambda\alpha_t)\beta_t}_{\beta_{t+1}} \left(\underbrace{z^t - \frac{\alpha_t \ell'(\beta_t \langle z^t, x^i \rangle, y^i)}{(1 - \lambda\alpha_t)\beta_t} x^i}_{z^{t+1}} \right)
\end{aligned}$$

$$\beta_{t+1} = (1 - \lambda\alpha_t)\beta_t, \qquad z^{t+1} = z^t - \frac{\alpha_t \ell'(\beta_t \langle z^t, x^i \rangle, y^i)}{(1 - \lambda\alpha_t)\beta_t} x^i$$

Lazy SGD updates for Sparse Data

SGD step

$$w^{t+1} = (1 - \lambda\alpha_t)w^t - \alpha_t \ell'(\langle w^t, x^i \rangle, y^i) x^i$$

EXE: re-write the iterates using $w^t = \beta_t z^t$ where $\beta_t \in \mathbb{R},\ z^t \in \mathbb{R}^d$

Can you update β_t and z^t so that each iteration is $O(s)$?

$$\beta_{t+1} z^{t+1} = (1 - \lambda\alpha_t)\beta_t z^t - \alpha_t \ell'(\beta_t \langle z^t, x^i \rangle, y^i) x^i$$

$$= \underbrace{(1 - \lambda\alpha_t)\beta_t}_{\beta_{t+1}} \left(\underbrace{z^t - \frac{\alpha_t \ell'(\beta_t \langle z^t, x^i \rangle, y^i)}{(1 - \lambda\alpha_t)\beta_t} x^i}_{z^{t+1}} \right)$$

O(1) scaling + *O(s)* sparse add = *O(s)* update

$$\beta_{t+1} = (1 - \lambda\alpha_t)\beta_t, \quad z^{t+1} = z^t - \frac{\alpha_t \ell'(\beta_t \langle z^t, x^i \rangle, y^i)}{(1 - \lambda\alpha_t)\beta_t} x^i$$

Part IV: Momentum

Issue with Gradient Descent

Solving the *training problem*: $\min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} f_i(w) =: f(w)$

Baseline method: Gradient Descent (GD)

$$w^{t+1} = w^t - \gamma \nabla f(w^t)$$

Step size/
Learning rate

Why GD and the Issues

Local rate of change

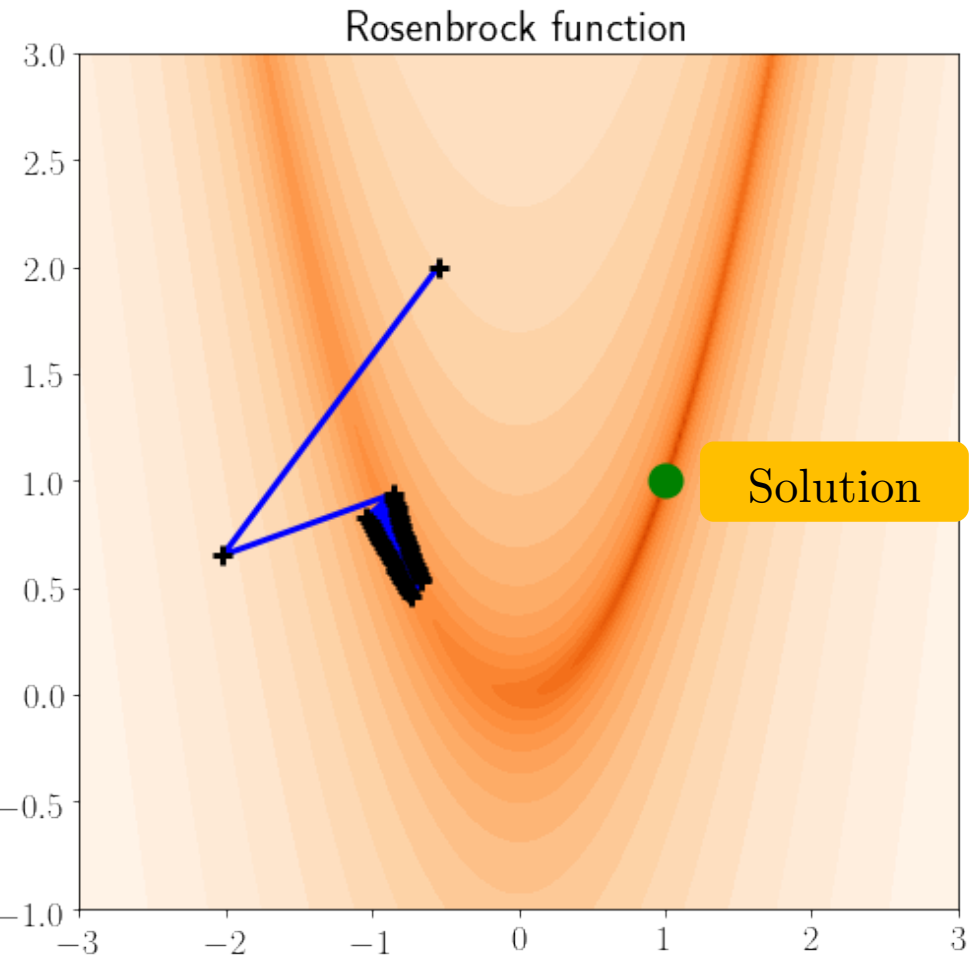
$$\Delta(d) := \lim_{s \to 0^+} \frac{f(x + ds) - f(x)}{s}$$

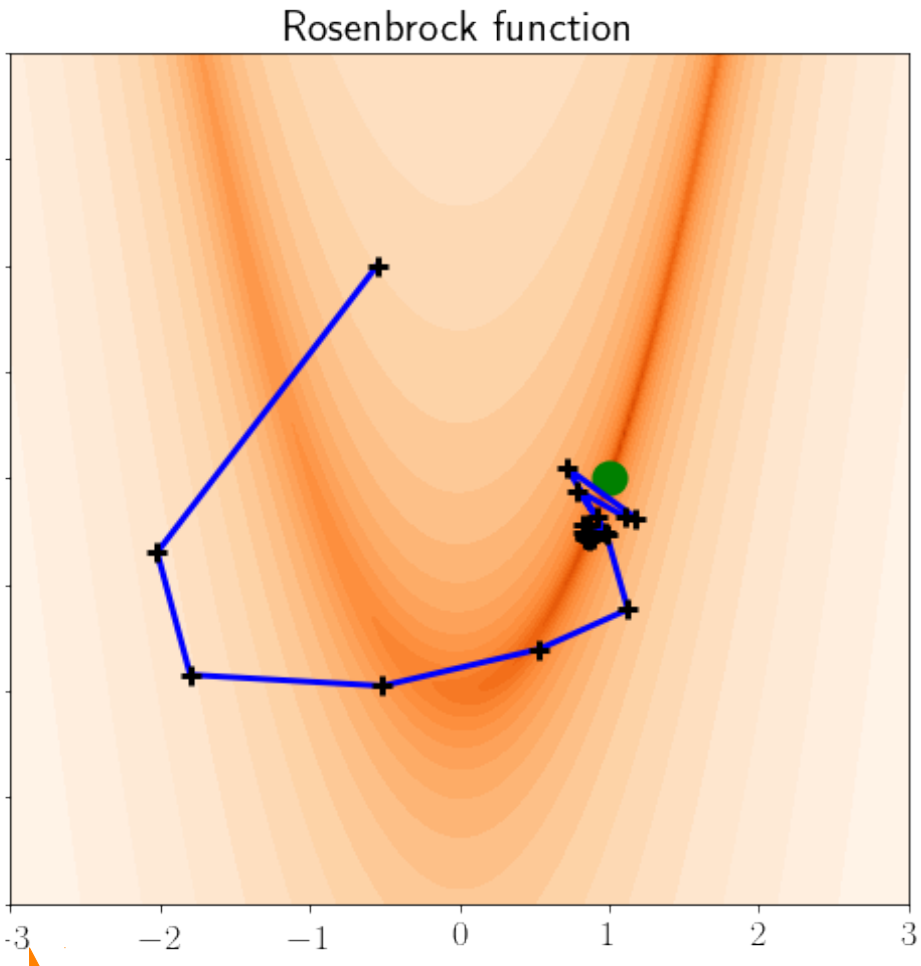
Max local rate

$$\frac{\nabla f(w^t)}{\|\nabla f(w^t)\|} := \max_{w \in \mathbb{R}^d} \Delta(d) \quad \text{subject to} \quad \|d\| = 1$$

GD is the "steepest descent"

Issue with Gradient Descent

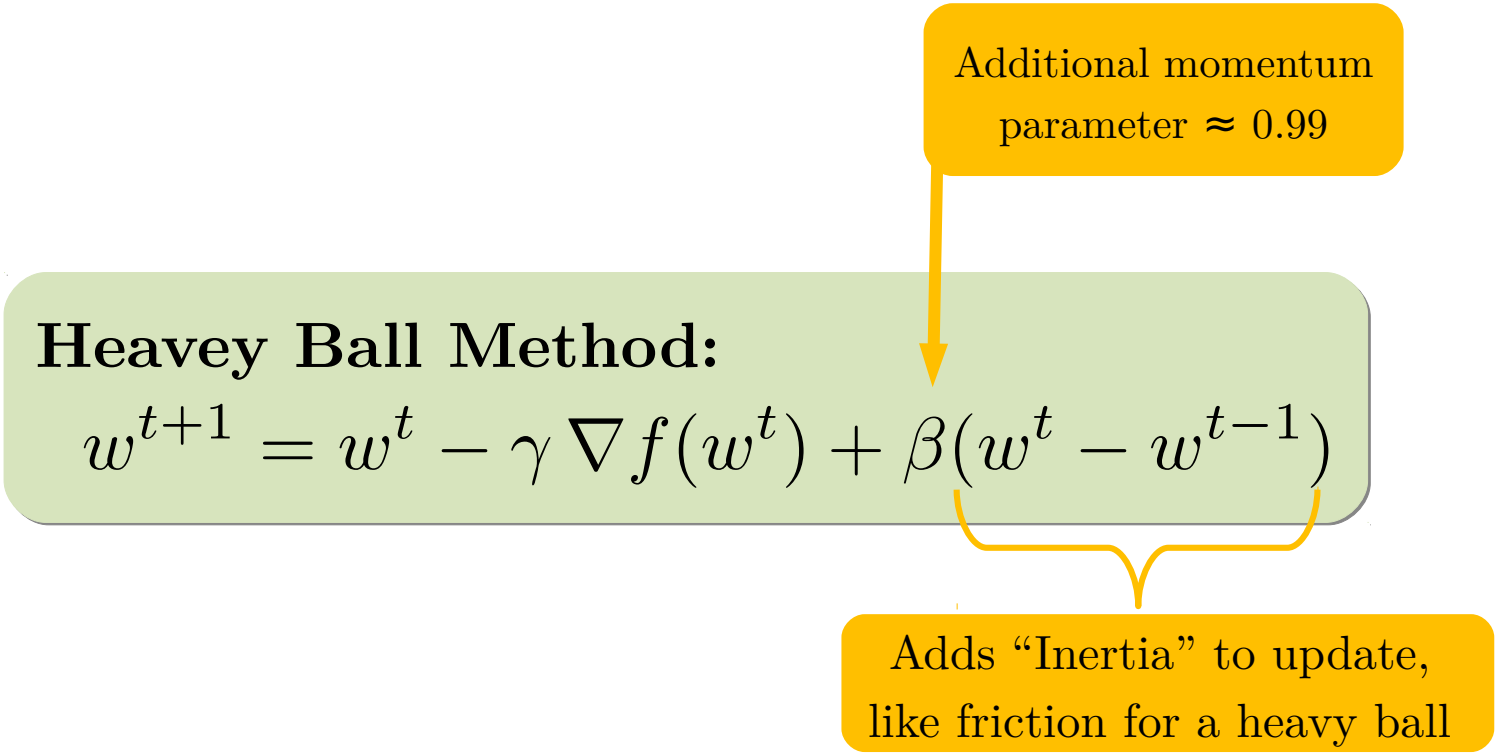




Get's stuck in "flat" valleys

Give momentum to keep going

Adding Momentum to GD

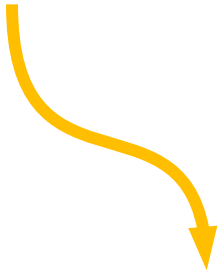


Equivalent Momentum formulation

Heavey Ball Method:

$$w^{t+1} = w^t - \gamma \nabla f(w^t) + \beta(w^t - w^{t-1})$$

Adds “Inertia” to update



Equivalent Momentum formulation

Heavey Ball Method:

$$w^{t+1} = w^t - \gamma \nabla f(w^t) + \beta(w^t - w^{t-1})$$

Adds "Inertia" to update

Adds "Momentum" to update

GD with momentum (GDm):

$$m^t = \beta\, m^{t-1} + \nabla f(w^t)$$

$$w^{t+1} = w^t - \gamma\, m^t$$

Equivalent Momentum formulation

GD with momentum:

$$m^t = \beta\, m^{t-1} + \nabla f(w^t)$$

$$w^{t+1} = w^t - \gamma\, m^t$$

Equivalent Momentum formulation

GD with momentum:

$$m^t = \beta\, m^{t-1} + \nabla f(w^t)$$
$$w^{t+1} = w^t - \gamma\, m^t$$

$$\begin{aligned} w^{t+1} &= w^t - \gamma\, m^t \\ &= w^t - \gamma\,(\beta m^{t-1} + \nabla f(w^t)) \\ &= w^t - \gamma\,\nabla f(w^t) - \gamma\beta\, m^{t-1} \\ &= w^t - \gamma\,\nabla f(w^t) + \frac{\gamma\beta}{\gamma}\,(w^t - w^{t-1}) \end{aligned}$$

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$$m^{t-1} = -\frac{1}{\gamma}(w^t - w^{t-1})$$

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$$m^{t-1} = -\frac{1}{\gamma}(w^t - w^{t-1})$$

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Equivalent Momentum formulation

GD with momentum:

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$$m^{t-1} = -\frac{1}{\gamma}(w^t - w^{t-1})$$

Heavey Ball Method:

$$w^{t+1} = w^t - \gamma\,\nabla f(w^t) + \beta(w^t - w^{t-1})$$

Equivalent Iterate Averaging formulation

Heavey Ball Method:

$$w^{t+1} = w^t - \gamma \nabla f(w^t) + \beta(w^t - w^{t-1})$$

Adds "Inertia" to update

Additional sequence of variables

Let $\eta > 0, \alpha \in [0, 1]$

New parameters

Averaging of variables

Equivalent Iterate Averaging formulation

Heavey Ball Method:

$$w^{t+1} = w^t - \gamma \nabla f(w^t) + \beta(w^t - w^{t-1})$$

Adds "Inertia" to update

Additional sequence of variables

Iterate Averaging: Let $\eta > 0, \alpha \in [0, 1]$

$$z_k = z_{k-1} - \eta \nabla f(x_k)$$

$$x_{k+1} = \frac{\alpha}{\alpha + 1} x_k + \frac{1}{\alpha + 1} z_k$$

New parameters

Averaging of variables

Convergence of Gradient Descent with Momentum

Polyak 1964

Theorem Let f be μ–strongly convex and L–smooth, that is

$$\mu I \preceq \nabla^2 f(w) \preceq LI, \quad \forall w \in \mathbb{R}^d$$

stepsize

If $\gamma = \dfrac{4}{(\sqrt{L}+\sqrt{\mu})^2}$ and $\beta = \dfrac{\sqrt{L}-\sqrt{\mu}}{\sqrt{L}+\sqrt{\mu}}$ then SGDm converges

momentum parameter

$$\|w^t - w^*\| \leq \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^t \|w^0 - w^*\|$$

$\kappa := L/\mu$

Convergence of Gradient Descent with Momentum

Polyak 1964

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stepsize

If $\gamma = \dfrac{4}{(\sqrt{L}+\sqrt{\mu})^2}$ and $\beta = \dfrac{\sqrt{L}-\sqrt{\mu}}{\sqrt{L}+\sqrt{\mu}}$ then SGDm converges

momentum parameter

$$\|w^t - w^*\| \leq \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^t \|w^0 - w^*\|$$

$\kappa := L/\mu$

Corollary $t \geq \dfrac{1}{\sqrt{\kappa}+1} \log\left(\dfrac{1}{\epsilon}\right)$ $\Rightarrow$ $\dfrac{\|w^t - w^*\|}{\|w^0 - w^*\|} \leq \epsilon$

Proof sketch: GDm convergence

Fundamental Theorem of Calculus

$$\int_{s=0}^{1} \nabla^2 f(w_s) ds (w^t - w^*) = \nabla f(w^t) - \nabla f(w^*) = \nabla f(w^t)$$

$w_s := w^* + s(w^t - w^*)$

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$$\begin{aligned} w^{t+1} - w^* &= w^t - w^* - \gamma \nabla f(w^t) + \beta(w^t - w^{t-1}) \\ &= \left(I - \gamma \int_{s=0}^{1} \nabla^2 f(w^s)\right)(w^t - w^*) + \beta(w^t - w^{t-1}) \\ &= \left((1+\beta)I - \gamma \int_{s=0}^{1} \nabla^2 f(w^s)\right)(w^t - w^*) - \beta(w^{t-1} - w^*) \end{aligned}$$

$+w^* - w^*$

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Depends on past. Difficult recurrence

Proof: Convergence of Heavy Ball

$$z^{t+1} = \begin{bmatrix} w^{t+1} - w^* \\ w^t - w^* \end{bmatrix} \in \mathbb{R}^{2d}$$

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EXE on Eigenvalues:

$$\text{If } \gamma = \frac{4}{(\sqrt{L}+\sqrt{\mu})^2} \text{ and } \quad \beta = \frac{\sqrt{L}-\sqrt{\mu}}{\sqrt{L}+\sqrt{\mu}} \text{ then}$$

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Adding Momentum to SGD

Rumelhart, Hinton, Geoffrey, Ronald, 1986, Nature

Stochastic Heavey Ball Method:

$$w^{t+1} = w^t - \gamma \nabla f_{j_t}(w^t) + \beta(w^t - w^{t-1})$$

Adds "Inertia" to update

SGD with momentum (SGDm):

$$m^t = \beta\, m^{t-1} + \nabla f_{j_t}(w^t)$$

$$w^{t+1} = w^t - \gamma\, m^t$$

Sampled i.i.d
$j \in \{1, \ldots, n\}$
$j \sim \frac{1}{n}$

SGDm and Averaging

$$
\begin{aligned}
m^t &= \beta\, m^{t-1} + \nabla f_{j_t}(w^t) \\
&= \beta\, m^{t-2} + \nabla f_{j_t}(w^t) + \beta \nabla f_{j_{t-1}}(w^{t-1}) \\
&= \sum_{i=1}^{t} \beta^i \nabla f_{j_{t-i}}(w^{t-i})
\end{aligned}
$$

http://fa.bianp.net/teaching/2018/COMP-652/stochastic_gradient.html

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Acts like an approximate variance reduction since

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Acts like an approximate variance reduction since

$$\sum_{i=1}^{t} \beta^i \nabla f_{j_{t-i}}(w^{t-i}) \approx \sum_{i=1}^{n} \frac{1}{n} \nabla f_i(w^t)$$

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