Optimization for Machine Learning Problems

Yan Yan

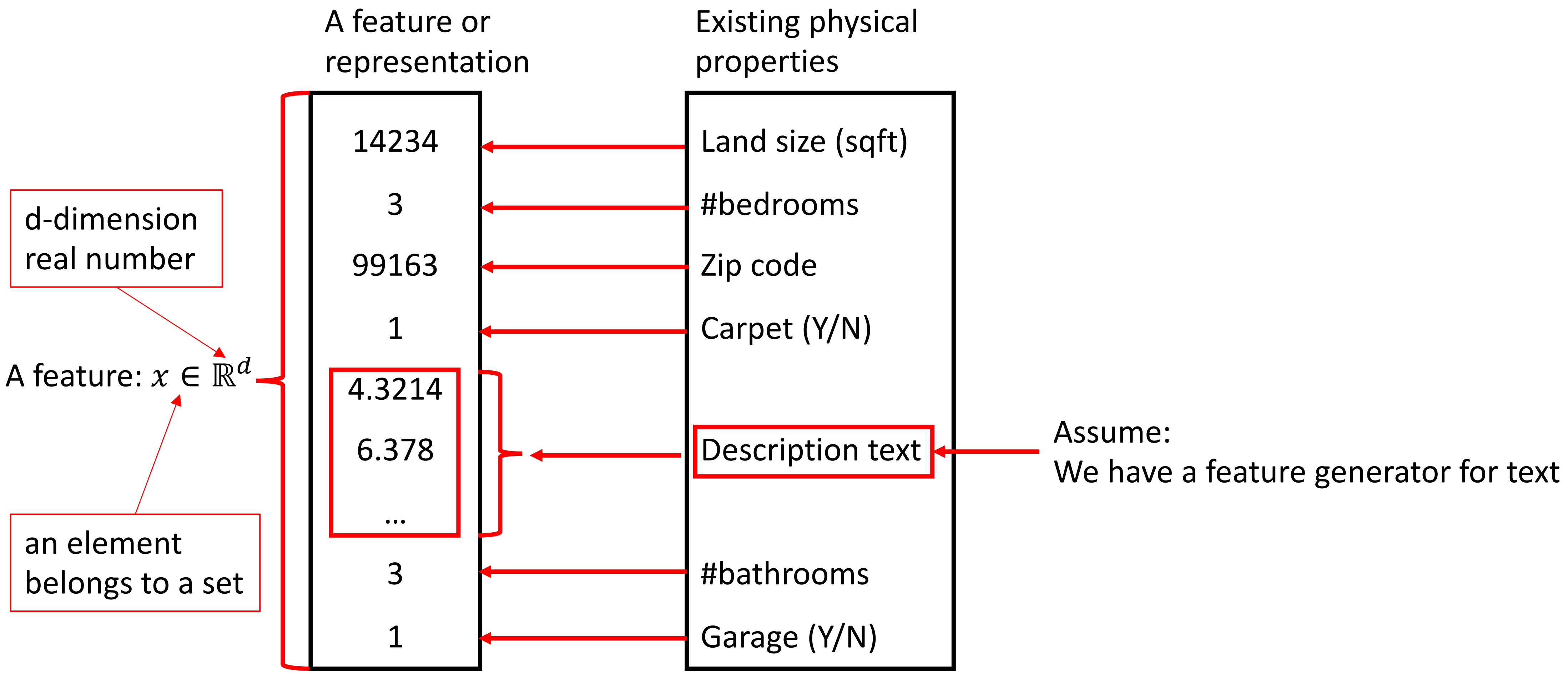
In last class

- Machine learning task details: classification, clustering and regression
    - Terminology
- Their connection to real world applications
    - Why we need these tools
- A showcase: how to construct a learning model
    - What can be used as features
    - Determine model structure
    - Determine model parameters

Today’s class includes

- Why is optimization important in machine learning (for determining model parameters)?
  - Efficiency of optimization algorithms
  - A showcase: the analytical solution VS gradient descent (GD)
- Common optimization algorithms
  - First-order algorithms
  - Second-order algorithms

House price model structure: linear model



Determining model parameters

- An optimization problem (on training set)

Objective function　　　　　　　　n training data

$$min_w f(w) = \frac{1}{n}\sum_{i=1}^{n} l(f(w; x_i), y_i) = \frac{1}{2n}\sum_{i=1}^{n}(x_i{}'w - y_i)^2$$

- 1-dimensional 1-data showcase with square loss

$$min_w \tfrac{1}{2}(wx - y)^2$$

- Analytical solution?

$$w^* = y/x$$

(first order optimality)

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- 1-dimensional multi-data square loss

$$min_w \frac{1}{2n}\sum_{i=1}^{n}(wx - y)^2$$

- Analytical solution?

$$w = \frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2}$$

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- multi-dimensional multi-data square loss

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$$\nabla_w f(w) = \frac{1}{n}\sum_{i=1}^{n} x_i{}'wx_i - y_i x_i \ \rightarrow \ 0$$

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- multi-dimensional multi-data square loss

$$min_w \frac{1}{2n}\sum_{i=1}^{n}(x_i{}'w - y_i)^2$$

$$X = [x_1, x_2, \dots, x_n] \in \mathbb{R}^{d\times n}$$

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \dots \\ y_n \end{bmatrix} \in \mathbb{R}^n$$

- Analytical solution?

$$\nabla_w f(w) = \frac{1}{n}\sum_{i=1}^{n} x_i{}'wx_i - y_i x_i \rightarrow 0 \Rightarrow XX'w^* - XY = 0$$

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$$\nabla_w f(w) = \frac{1}{n}\sum_{i=1}^{n} x_i{}'wx_i - y_i x_i \to 0 \Rightarrow XX'w^* - XY = 0 \Rightarrow w^* = (XX')^{-1}XY$$

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Q: is this closed form solution a good way in practice? Why?

Determining model parameters

- Computational complexity for the analytical solution?

$$\nabla_w f(w) = \frac{1}{n}\sum_{i=1}^{n} x_i{}' w x_i - y_i x_i \;\rightarrow\; 0 \quad \Rightarrow \quad XX'w^* - XY = 0 \quad \Rightarrow \quad w^* = (XX')^{-1}XY$$

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- Inverse of a scalar?

$$x\, x^{-1} = 1 \ \rightarrow x^{-1} = 1/x$$

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- Inverse of a scalar?

$$x\, x^{-1} = 1 \ \rightarrow x^{-1} = 1/x$$

- Inverse of a matrix?

$$XX^{-1} = I = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

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Matrix multiplication	One $n \times m$ matrix & one $m \times p$ matrix	One $n \times p$ matrix	Schoolbook matrix multiplication	$O(nmp)$

Screenshot from https://en.wikipedia.org/wiki/Computational_complexity_of_mathematical_operations#Matrix_algebra

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Matrix inversion*	One $n \times n$ matrix	One $n \times n$ matrix	Gauss–Jordan elimination	$O(n^3)$
			Strassen algorithm	$O(n^{2.807})$
			Coppersmith–Winograd algorithm	$O(n^{2.376})$
			Optimized CW-like algorithms	$O(n^{2.373})$

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Not every matrix has inversion

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- Matrix multiplication:

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- Matrix multiplication:

$$\boxed{XX'\text{: d×n×d}} \quad \boxed{XY\text{: d×n}} \quad \boxed{(XX')^{-1}XY: d \times d \times n} \rightarrow O(d^2 n)$$

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$$\boxed{XX': \mathrm{d}\times\mathrm{n}\times\mathrm{d}} \quad \boxed{XY: \mathrm{d}\times\mathrm{n}} \quad \boxed{(XX')^{-1}XY: d\times d\times n} \quad \rightarrow O(d^2 n)$$

- Inverse of a matrix:

$$(XX')^{-1}:\ O(d^{2.373})$$

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- Inverse of a matrix:

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- Total complexity

$$O(d^2 n + d^{2.373})$$

Determining model parameters

- Can Gradient Descent (GD) do better?

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$$\nabla_w f(w) = \frac{1}{n}\sum_{i=1}^{n} x_i' w x_i - y_i x_i \;\rightarrow\; O(dn)$$

$$w_{t+1} = w_t - \alpha_t \nabla_w f(w_t) \;\rightarrow\; O(d) \longrightarrow \text{An iterative algorithm}$$

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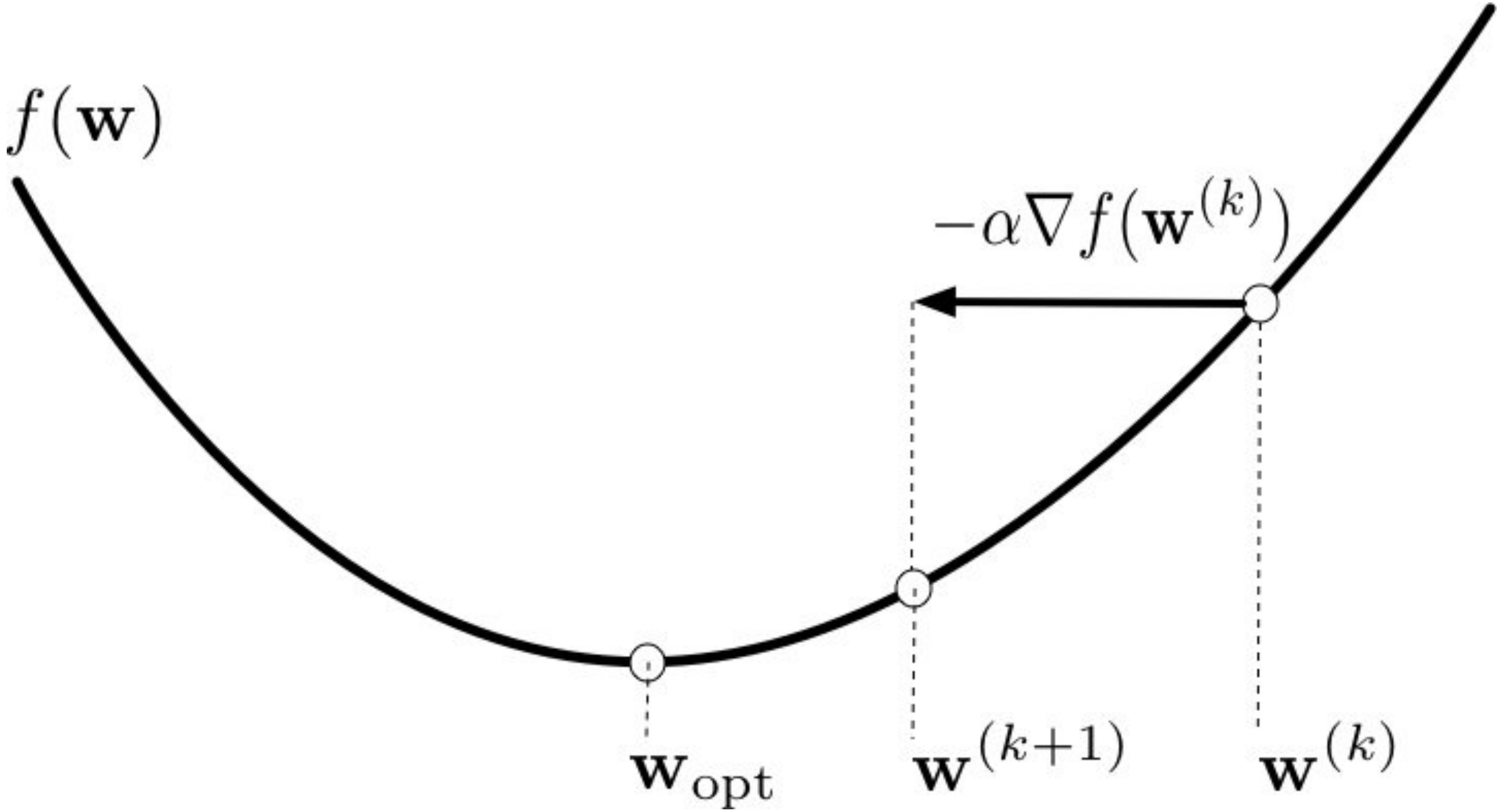
An iterative algorithm

Step size (learning rate): usually pre-defined


$f(\mathbf{w})$
$-\alpha \nabla f(\mathbf{w}^{(k)})$
$\mathbf{w}_{\mathrm{opt}}$
$\mathbf{w}^{(k+1)}$
$\mathbf{w}^{(k)}$

[Jung2018]

Determining model parameters

- Can Gradient Descent (GD) do better?

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$$O(dnT)$$

Determining model parameters

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$O(dnT)$ VS. $O(d^2 n + d^{2.373})$ for the closed form solution

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$T < d$: then GD has less computational complexity

Determining model parameters

- When to terminate GD (determining T)?
  - An approximated solution

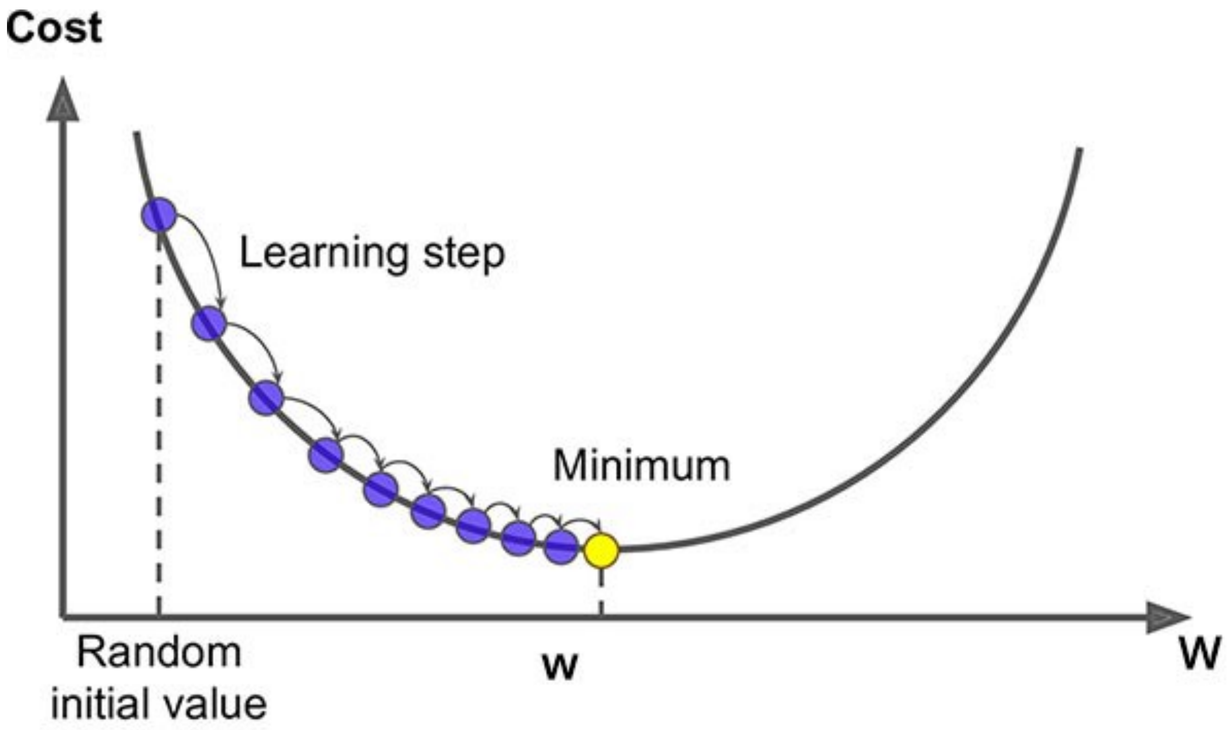
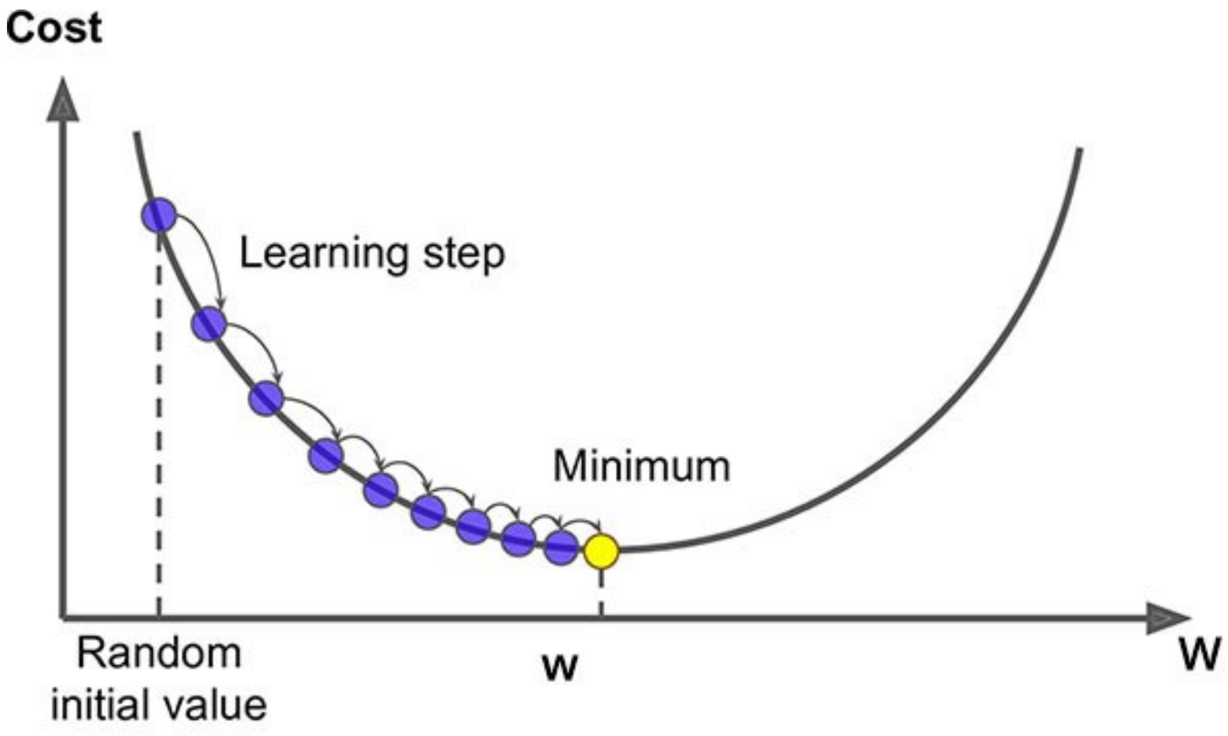


Image from https://morioh.com/p/15c995420be6

Determining model parameters

- When to terminate GD (determining T)?
  - An approximated solution: difficult to set up step size exactly to minimal solution(s)



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Determining model parameters

- When to terminate GD (determining T)?
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No need to know this solution
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Level of accuracy:
ϵ-accurate solution

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  - Convergence of GD?
    - When $T \to \infty$, then $\epsilon \to 0$
    - But: when to terminate GD?

Determining model parameters

- When to terminate GD (determining T)?
  - Provable convergence: rate of convergence
    - If ϵ is a function of T: $\epsilon(\mathrm{T})$
    - Larger T $\rightarrow$ smaller $\epsilon(\mathrm{T})$

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    - If determining $\epsilon(\mathrm{T})$ theoretically:

      we know roughly when to terminate optimization algorithm

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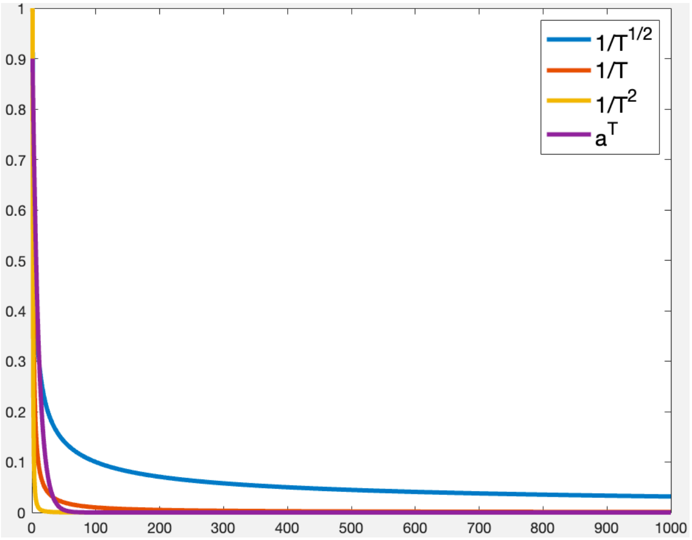

$$\epsilon(\mathrm{T}) = \frac{1}{\sqrt{T}}$$

$$\epsilon(\mathrm{T}) = \frac{1}{T}$$

$$\epsilon(\mathrm{T}) = \frac{1}{T^2}$$

$$\epsilon(\mathrm{T}) = a^T \qquad a = 0.9$$

Determining model parameters

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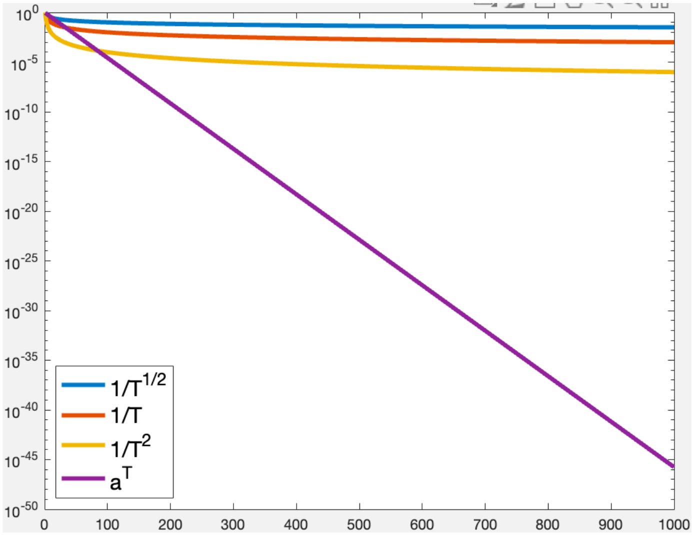

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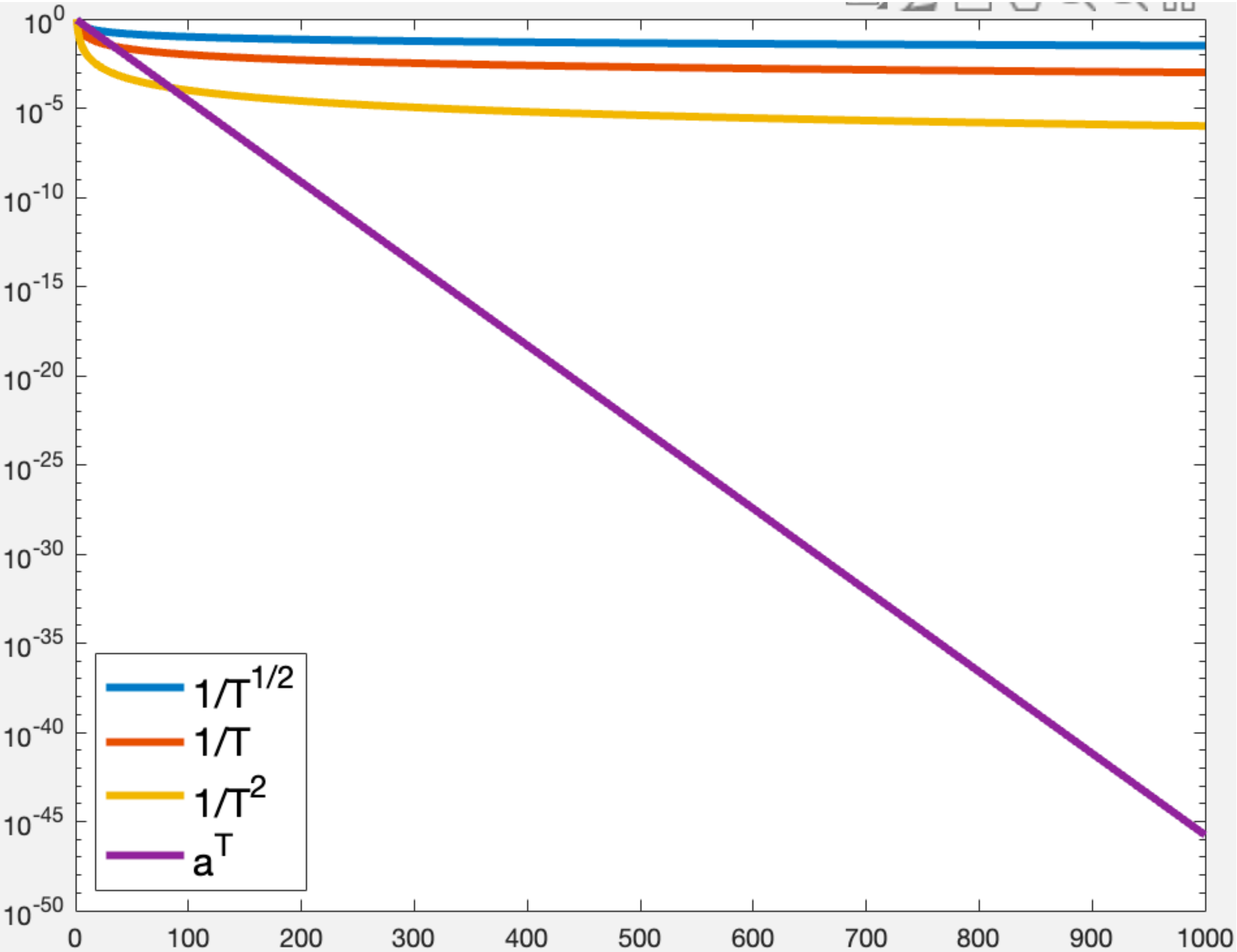

10^0
10^-5
10^-10
10^-15
10^-20
10^-25
10^-30
10^-35
10^-40
10^-45
10^-50
0
100
200
300
400
500
600
700
800
900
1000
1/T^1/2
1/T
1/T^2
a^T

Determining model parameters

- When to terminate GD (determining T)?
  - Main factors influencing convergence rate?
    - Step size (learning rate)

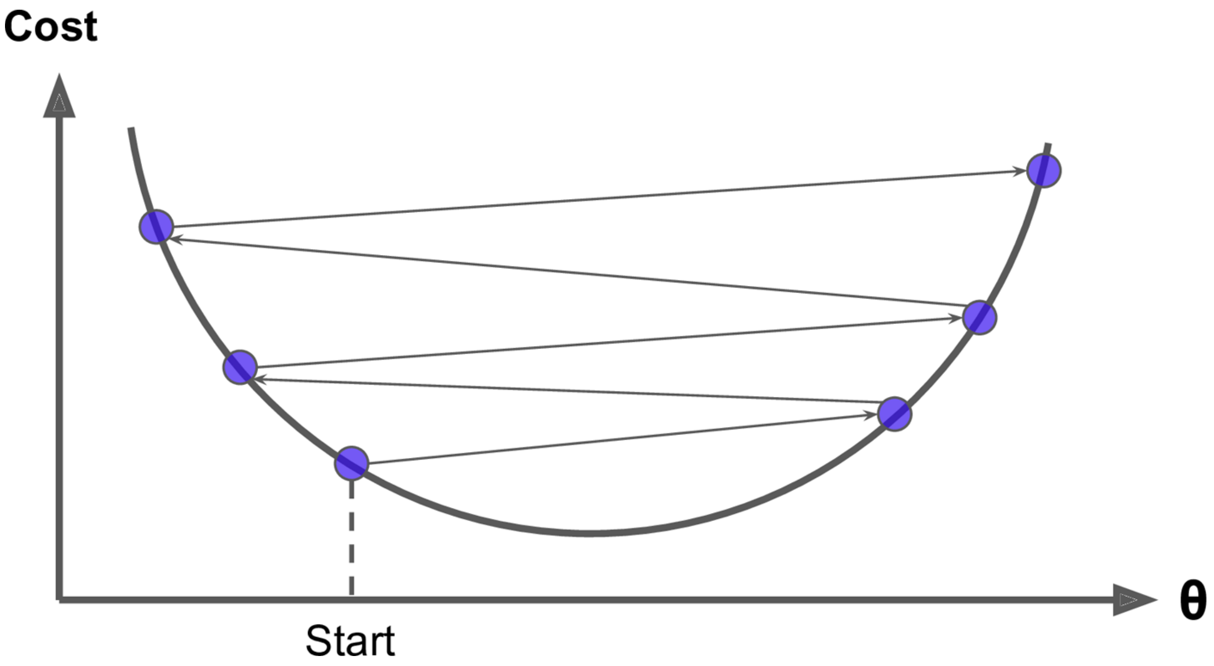

Image from https://www.oreilly.com/library/view/hands-on-machine-learning/9781491962282/ch04.html

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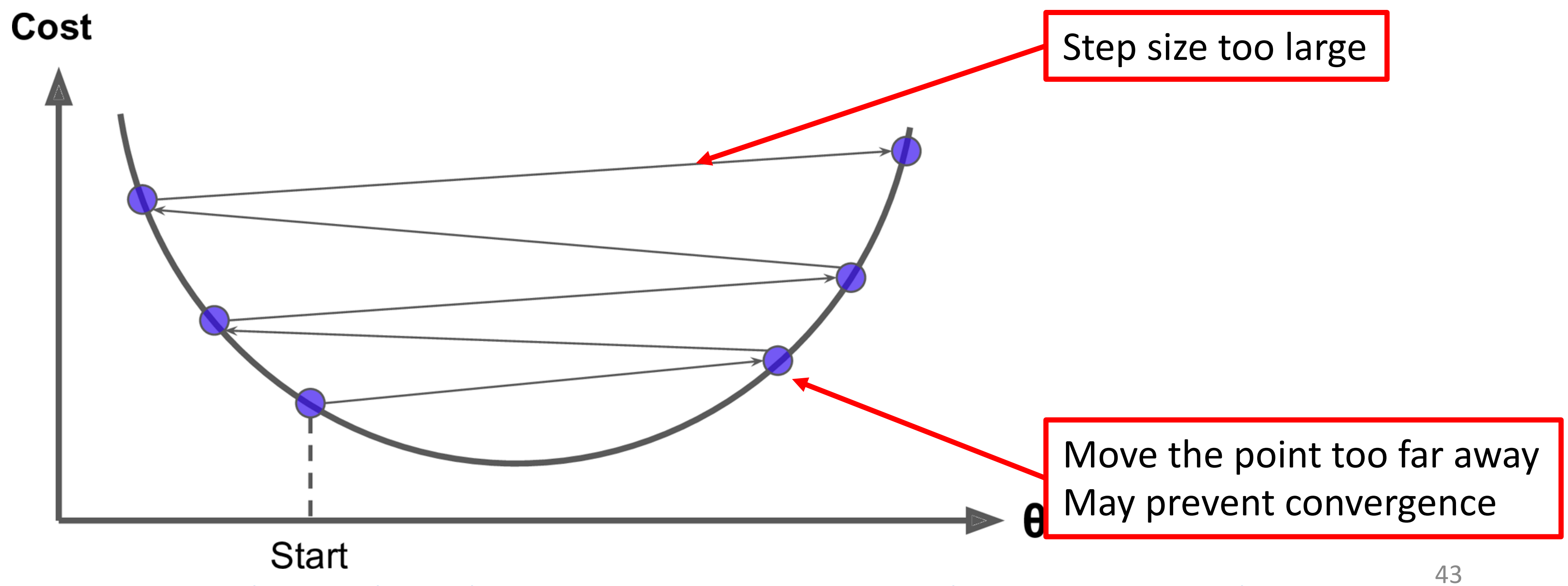

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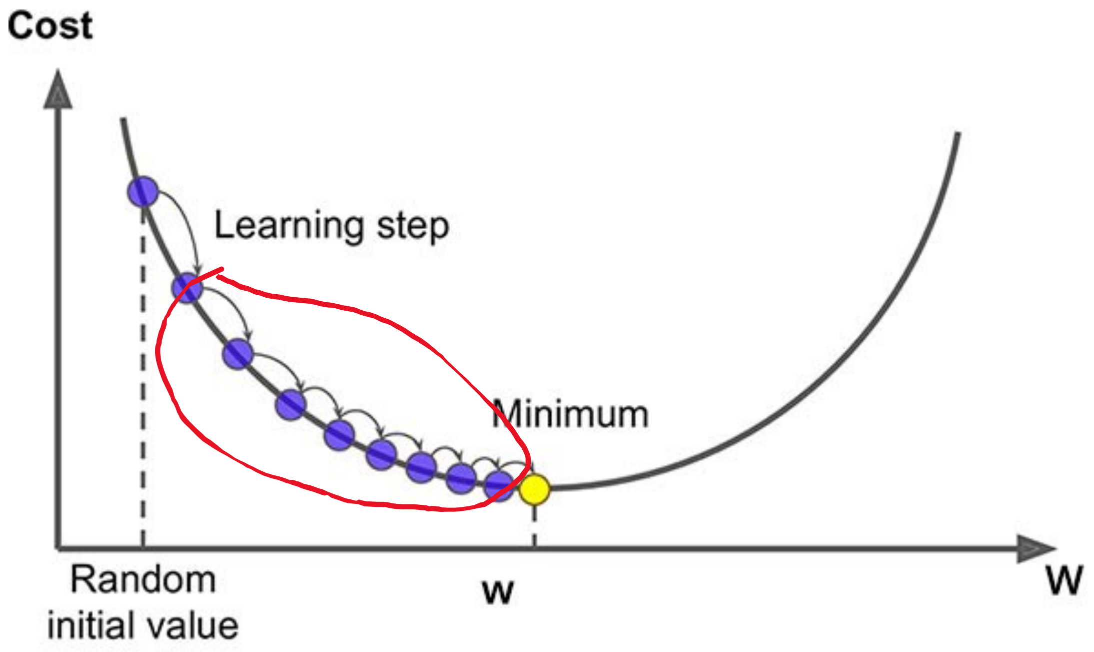

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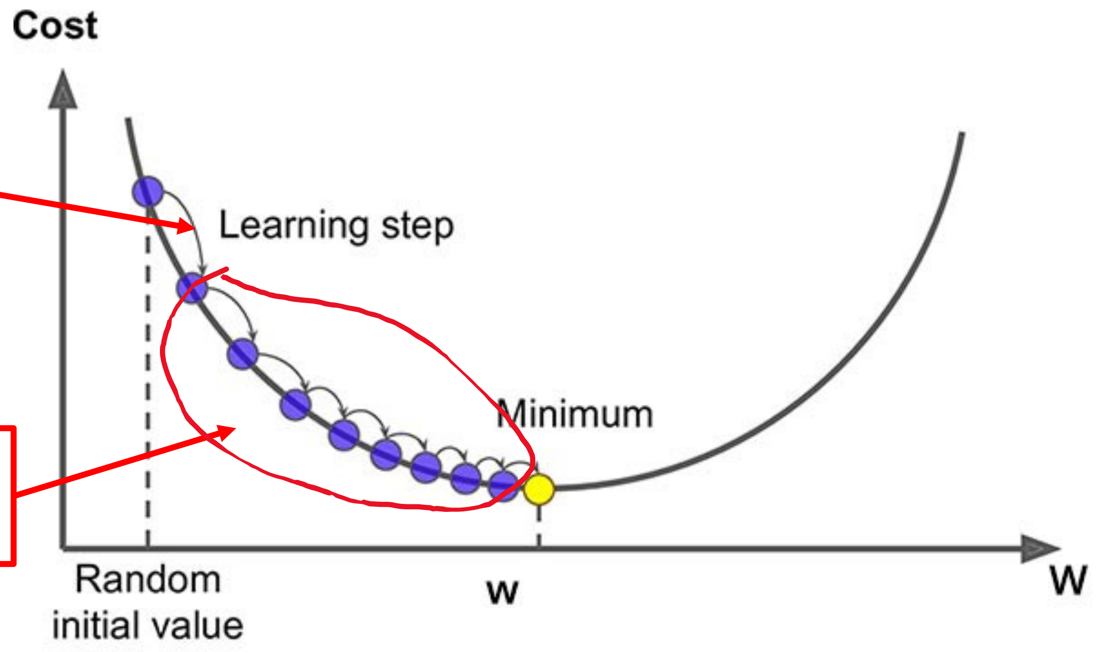
Step size too small

May cost too many steps approaching the minimal solution



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Determining model parameters

- When to terminate GD (determining T)?
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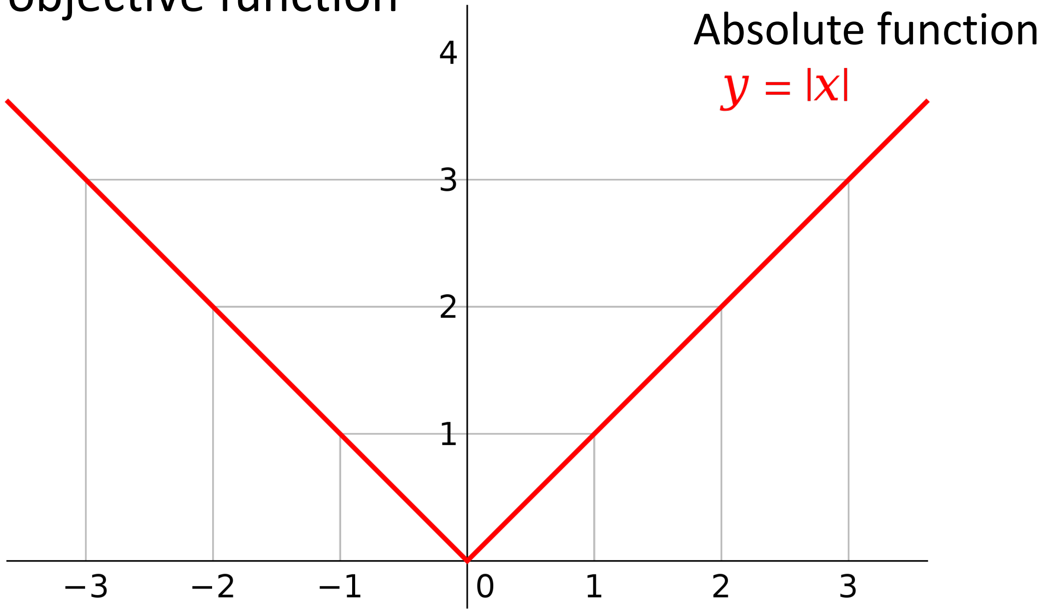

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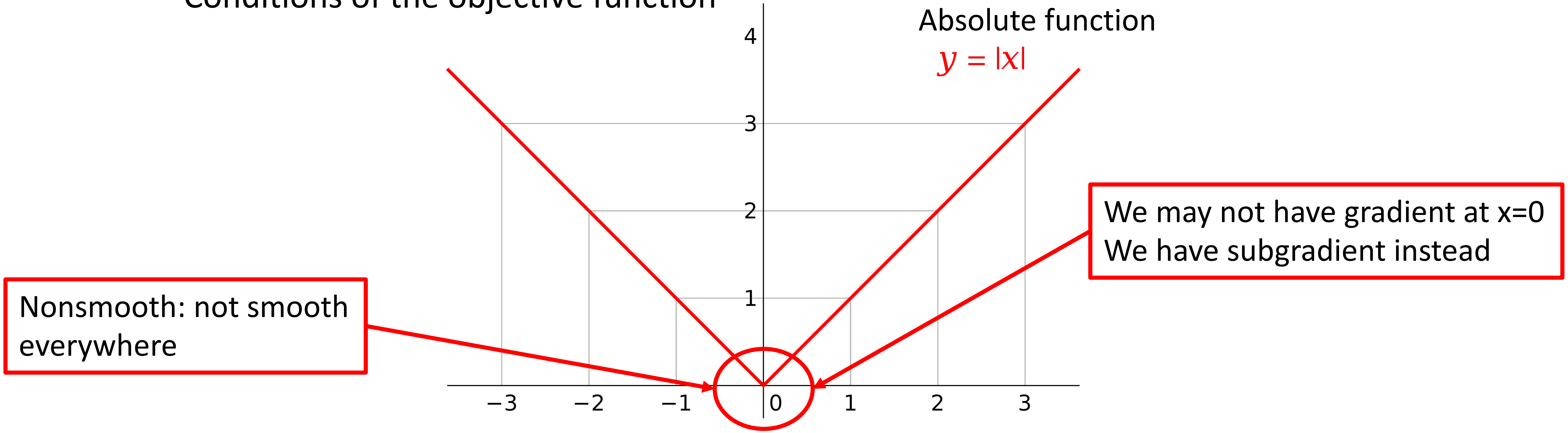

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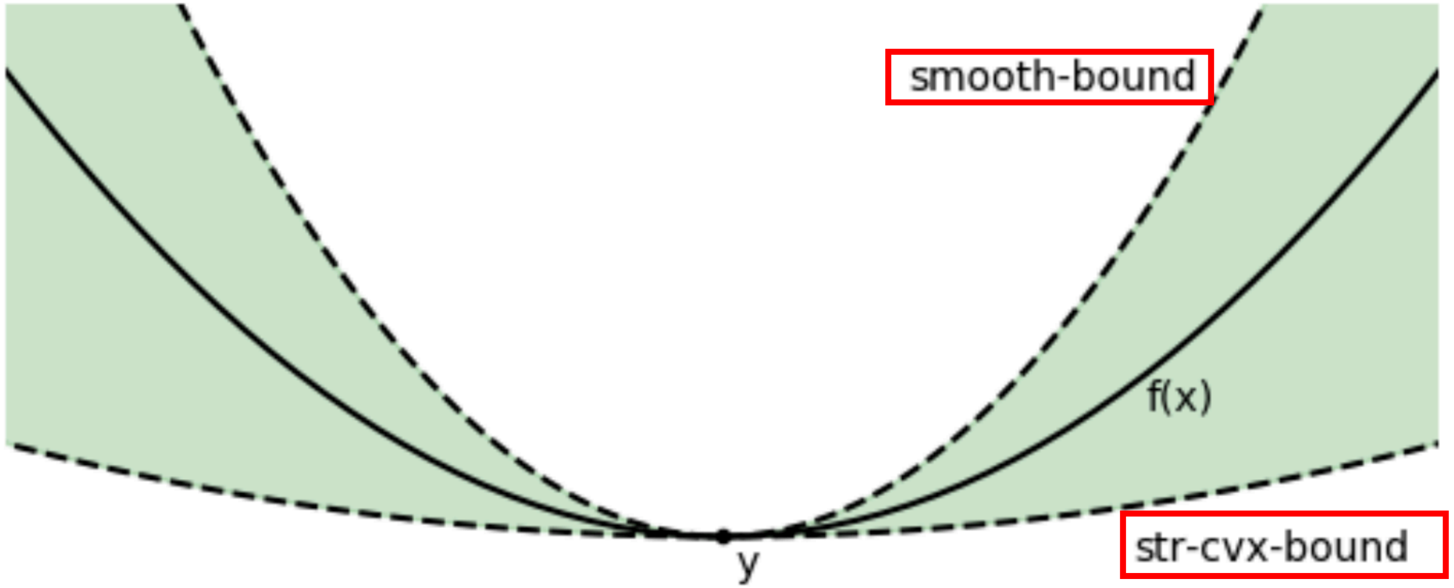

Image from IFT 6085 - Lecture 3 Gradients for smooth and for strongly convex functions
http://mitliagkas.github.io/ift6085-2019/ift-6085-lecture-3-notes.pdf

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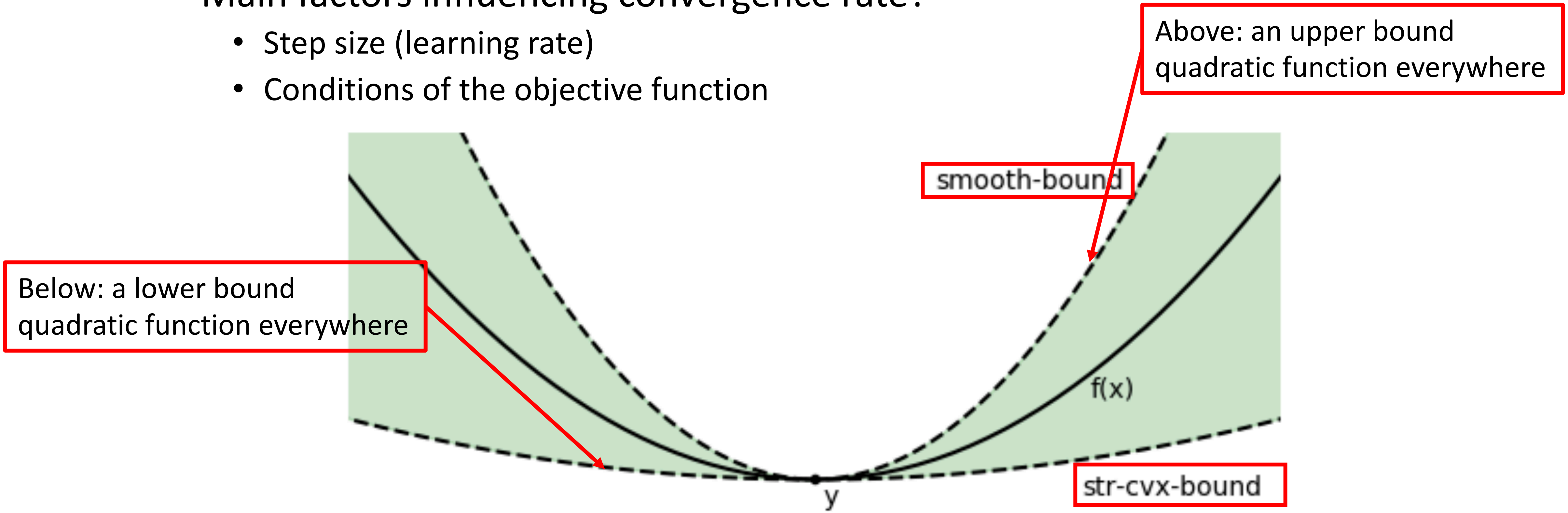

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  - Come back to our problem setting:
    Convergence rate for GD?

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Theorem 2.1.14 *If* $f \in \mathcal{S}^{1,1}_{\mu,L}(R^n)$ *and* $0 < h \leq \frac{2}{\mu+L}$ *then the gradient method generates a sequence* $\{x_k\}$ *such that*

$$\| x_k - x^* \|^2 \leq \left(1 - \frac{2h\mu L}{\mu + L}\right)^k \| x_0 - x^* \|^2 .$$

If $h = \frac{2}{\mu+L}$ *then*

$$\| x_k - x^* \| \leq \left(\frac{Q_f-1}{Q_f+1}\right)^k \| x_0 - x^* \|,$$

$$f(x_k) - f^* \leq \frac{L}{2}\left(\frac{Q_f-1}{Q_f+1}\right)^{2k} \| x_0 - x^* \|^2,$$

where $Q_f = L/\mu$.

[Nesterov 2003]

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    Convergence rate for GD?

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$$\| x_k - x^* \|^2 \leq \left(1 - \frac{2h\mu L}{\mu + L}\right)^k \| x_0 - x^* \|^2 .$$

If $h = \frac{2}{\mu+L}$ *then*

$$\| x_k - x^* \| \leq \left(\frac{Q_f - 1}{Q_f + 1}\right)^k \| x_0 - x^* \|,$$

$$f(x_k) - f^* \leq \boxed{\frac{L}{2}\left(\frac{Q_f - 1}{Q_f + 1}\right)^{2k} \| x_0 - x^* \|^2,} \quad \boxed{= \epsilon(\mathrm{k}) = O(a^k)}$$

where $Q_f = L/\mu$.

[Nesterov 2003]

Determining model parameters

- When to terminate GD (determining T)?
  - Come back to our problem setting:
    Convergence rate for GD?

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$$\boxed{k = O(\, log_{1/a}(1/\epsilon))}$$

where $Q_f = L/\mu$.

[Nesterov 2003]

Determining model parameters

- Now we can answer the question:

  Can Gradient Descent (GD) do better?

GD	vs	Analytical solution
$O(dnT)$		$O(d^2n + d^{2.373})$

Determining model parameters

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$$\boxed{\begin{array}{c}\text{GD}\\ O(dnT)\end{array}} \quad \text{VS} \quad \boxed{\begin{array}{c}\text{Analytical solution}\\ O(d^2n + d^{2.373})\end{array}}$$

$$\downarrow$$

$$\boxed{O(dn{\times}log_{1/a}(1/\epsilon))}$$

Determining model parameters

- Is log term $log_{1/a}(1/\epsilon)$ large?

Determining model parameters

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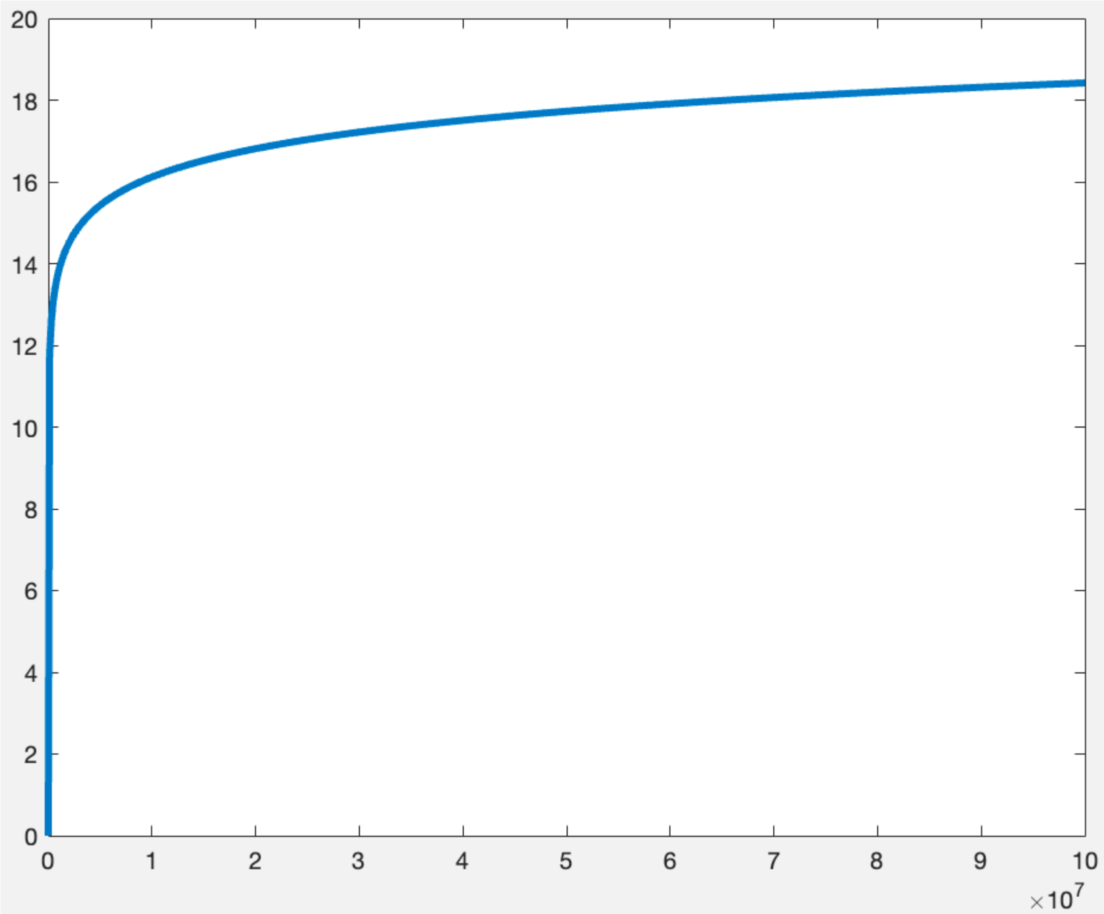

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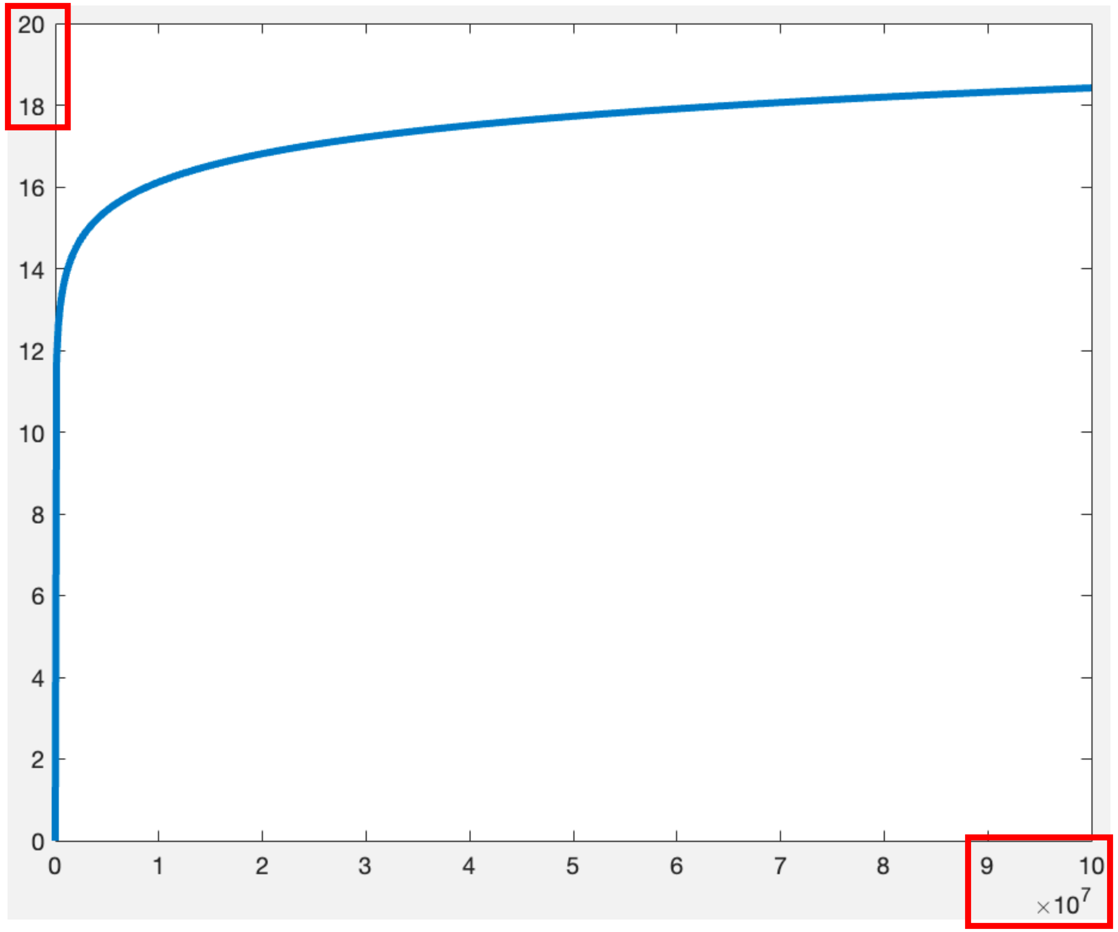

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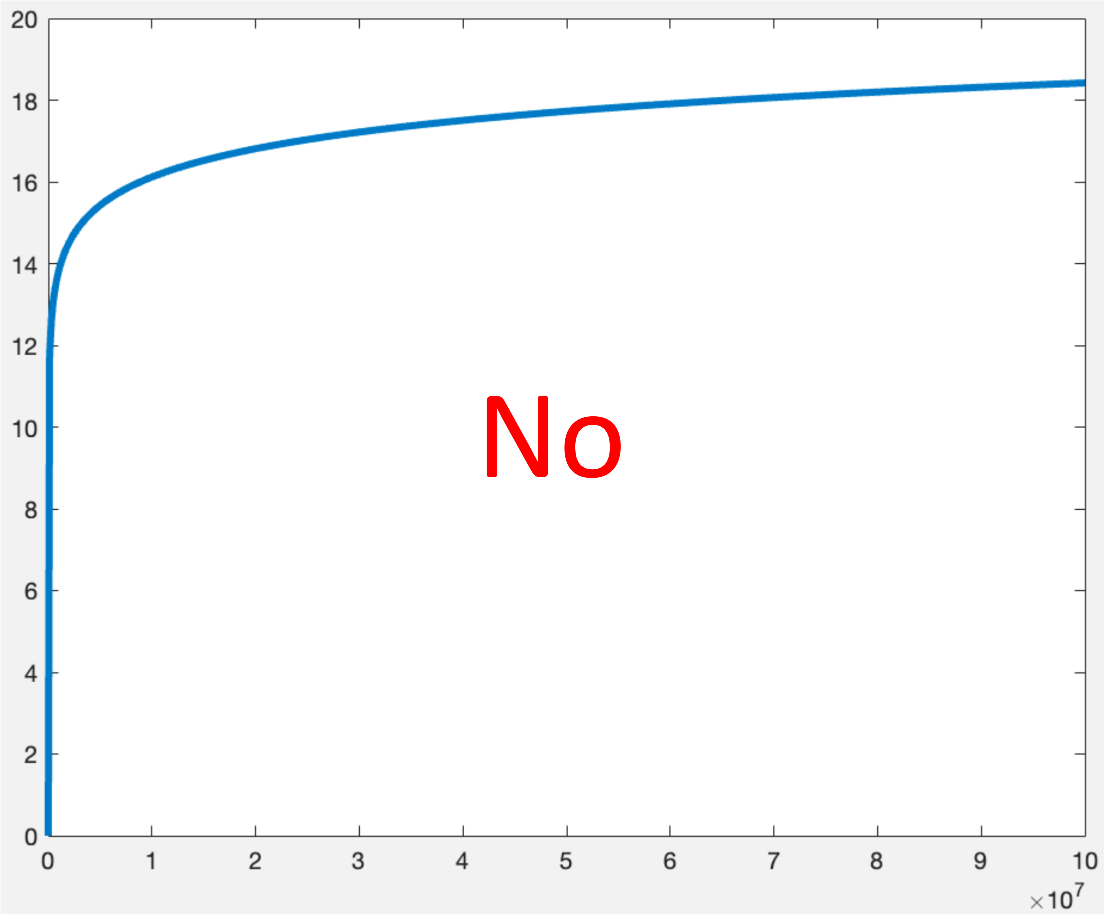

Determining model parameters

- Is d large?

Screenshot from https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/

name	source	type	class	training size	testing size	feature
a1a	UCI	classification	2	1,605	30,956	123
a2a	UCI	classification	2	2,265	30,296	123
a3a	UCI	classification	2	3,185	29,376	123
a4a	UCI	classification	2	4,781	27,780	123
a5a	UCI	classification	2	6,414	26,147	123
a6a	UCI	classification	2	11,220	21,341	123
a7a	UCI	classification	2	16,100	16,461	123
a8a	UCI	classification	2	22,696	9,865	123
a9a	UCI	classification	2	32,561	16,281	123
australian	Statlog	classification	2	690		14
avazu	Avazu's Click-through Prediction	classification	2	40,428,967	4,577,464	1,000,000
breast-cancer	UCI	classification	2	683		10
cod-rna	[AVU06a]	classification	2	59,535		8
colon-cancer	[AU99a]	classification	2	62		2,000
covtype.binary	UCI	classification	2	581,012		54
criteo	Criteo's Display Advertising Challenge	classification	2	45,840,617	6,042,135	1,000,000
criteo_tb	Criteo's Terabyte Click Logs	classification	2	4,195,197,692	178,274,637	1,000,000
diabetes	UCI	classification	2	768		8
duke breast-cancer	[MW01a]	classification	2	44		7,129
epsilon	PASCAL Challenge 2008	classification	2	400,000	100,000	2,000
fourclass	[TKH96a]	classification	2	862		2
german.numer	Statlog	classification	2	1,000		24
gisette	NIPS 2003 Feature Selection Challenge [IG05a]	classification	2	6,000	1,000	5,000
heart	Statlog	classification	2	270		13
HIGGS	UCI	classification	2	11,000,000		28
ijcnn1	[DP01a]	classification	2	49,990	91,701	22
ionosphere	UCI	classification	2	351		34
kdd2010 (algebra)	KDD CUP 2010	classification	2	8,407,752	510,302	20,216,830
kdd2010 (bridge to algebra)	KDD CUP 2010	classification	2	19,264,097	748,401	29,890,095
kdd2010 raw version (bridge to algebra)	KDD CUP 2010	classification	2	19,264,097	748,401	1,163,024
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1,000,000

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Determining model parameters

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  Yes!

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GD	vs	Analytical solution
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Determining model parameters

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GD
$O(dnT)$

VS

Analytical solution
$O(d^2n + d^{2.373})$

$O(dn \times log_{1/a}(1/\epsilon))$

Determining model parameters

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GD
$O(dnT)$

$O(dn \times log_{1/a}(1/\epsilon))$

vs

Analytical solution
$O(d^2n + d^{2.373})$

If:
$n = 10^8$
$d = 10^6$

Determining model parameters

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GD
$O(dnT)$

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Analytical solution
$O(d^2n + d^{2.373})$

$O(dn \times log_{1/a}(1/\epsilon))$

If:
$n = 10^8$
$d = 10^6$

$(10^6)^2 \times 10^8 - 10^6 \times 10^8 = 10^{20} - 10^{14}$

Determining model parameters

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vs

Analytical solution

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$O(d^2n + d^{2.373})$

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If:
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$(10^6)^2 \times 10^8 - 10^6 \times 10^8 = 10^{20} - 10^{14} \approx 10^{20}$

$O\left(dn \times log_a\left(\frac{1}{\epsilon}\right)\right) \ll O(d^2n + n^{2.373})$

Other optimization algorithms

- First-order algorithms
  - Gradient descent
  - Momentum methods
  - Stochastic variants
  - Hessian vector products
- Second-order algorithms
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References

- Jung, Alexander. (2018). Machine Learning: Basic Principles.
- Nesterov, Yurii. *Introductory lectures on convex optimization: A basic course*. Vol. 87. Springer Science & Business Media, 2003.