CS4641 Spring 2025
Linear Regression

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Teaching Assistants

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Office Hours

Tuesday: 2:30-3:30pm, *Online* (Join Session): Prof. Dai

Wednesday: 3:00-4:00pm, *Coda**: Haotian Sun, Zihao Zhao, Jonathan Li

Friday: 3:00-4:00pm, *Coda**: Tianyi Chen, Binyue Deng

***Note:** "Coda" refers to the second floor of the Coda building, shared area near the escalator.

Organization

- *Background knowledge*
  - Probability and Statistics, Linear Algebra, Optimization, Coding skills
- *Supervised learning*
- *Unsupervised learning*
- *Advanced Topics*

Syllabus

- *Background knowledge*
    - Probability and Statistics, Linear Algebra, Optimization, Coding skills
- *Supervised learning*
- *Unsupervised learning*
- *Advanced Topics*

Modeling: what to learn
Learning: how to learn
Implementation

Syllabus

- *Background knowledge*
  - Probability and Statistics, Linear Algebra, Optimization, Coding skills
- *Supervised learning*
- *Unsupervised learning*
- *Advanced Topics*

Modeling: Probability and Statistics, Linear Algebra
Learning: Optimization, Linear Algebra
Implementation: Coding

ML Algorithm Pipeline

General ML Algorithm Pipeline

1. Build probabilistic models
2. Derive loss function (by MLE or MAP)
3. Select optimizer

Syllabus

- *Background knowledge*
  - Probability and Statistics, Linear Algebra, Optimization, Coding skills
- *Supervised learning*
- *Unsupervised learning*
- *Advanced Topics*

Modeling: Probability and Statistics, Linear Algebra
Learning: Optimization, Linear Algebra
Implementation: Coding

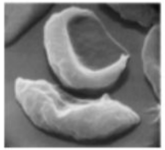
Supervised Learning

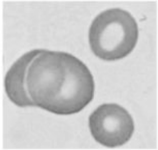
Classification

X = Document

Sports
Science
News

Y = Topic



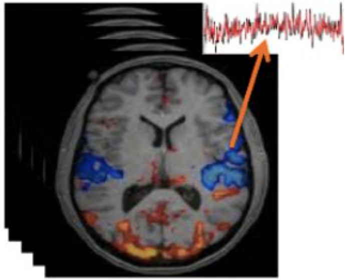


X = Cell Image

Anemic cell
Healthy cell

Y = Diagnosis

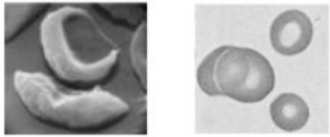
Regression



X = Brain Scan

Y = Age of a subject

Classification Tasks

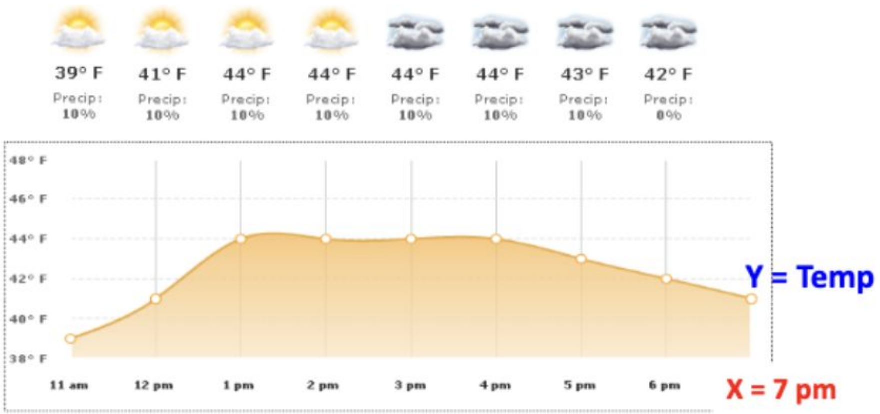
	Feature, X		Label, Y
Diagnosing sickle cell anemia		→	Anemic cell Healthy cell
Tax Fraud Detection	see table below	→	Cheat: ?
Web Classification		→	Sports Science News
Predict squirrel hill resident	Drive to CMU, Rachel's fan, Shop at SH Giant Eagle	→	Resident Not resident

Refund	Marital Status	Taxable Income
No	Married	80K

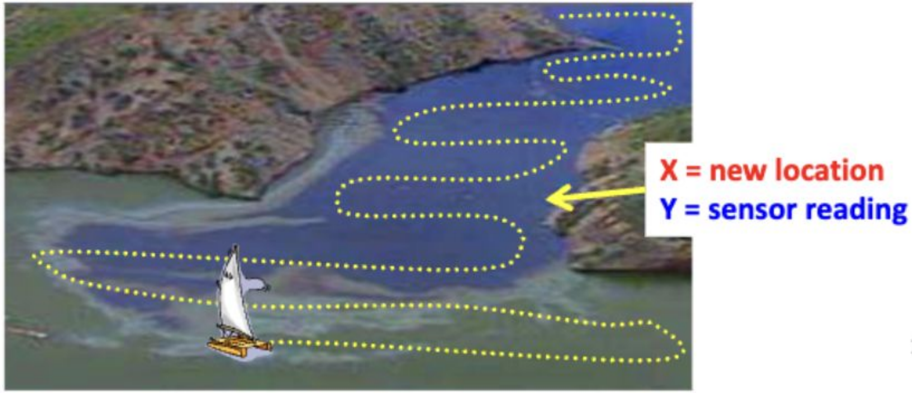
Cheat
?

Regression Tasks

Weather Prediction



Estimating Contamination

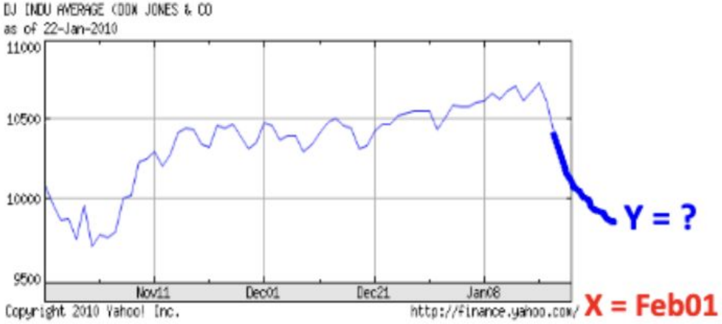


Supervised Learning

Goal: Construct a predictor f: X → Y to
minimize a risk (performance measure) R(f).

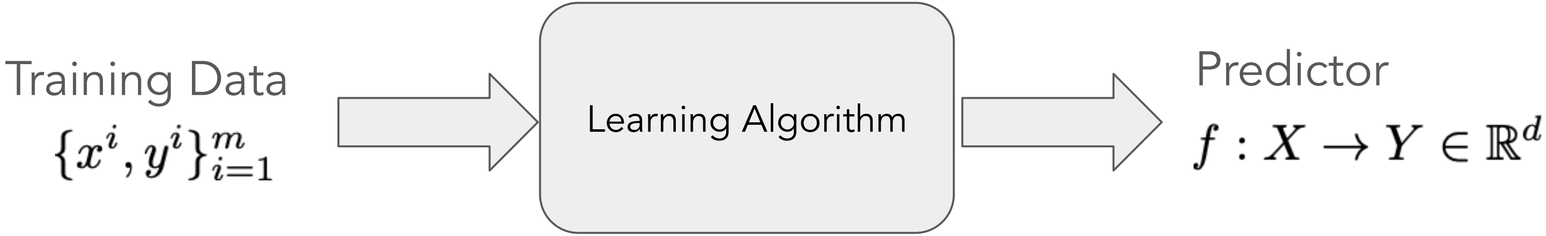
Sports
Science
News

Classification



Regression

Regression algorithms



Regression algorithms

Training Data $\{x^i, y^i\}_{i=1}^{m}$ → Learning Algorithm → Predictor $f : X \to Y \in \mathbb{R}^d$

Linear Regression

Regularized Linear Regression:

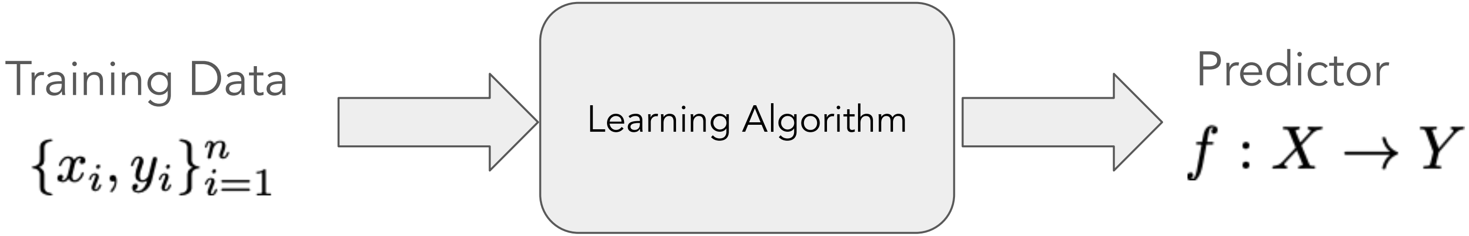
Ridge Regression, Lasso

Nonlinear Regression:

Kernel Regression, Neural Network

….

Regression algorithms



General ML Algorithm Pipeline

1. Build probabilistic models
2. Derive loss function (by MLE or MAP)
3. Select optimizer

Machine Learning for Apartment Hunting

- Suppose you are to move to Atlanta
- And you want to find the most reasonably priced apartment satisfying your needs:

Living area (ft^2)	# bedroom	Monthly rent ($)
230	1	900
506	2	1800
433	2	1500
190	1	800
…		
150	1	?
270	1.5	?

Regression algorithms

Training Data $\{x^i, y^i\}_{i=1}^m$ → Learning Algorithm → Predictor $f : X \to Y$

General ML Algorithm Pipeline

1. Build probabilistic models
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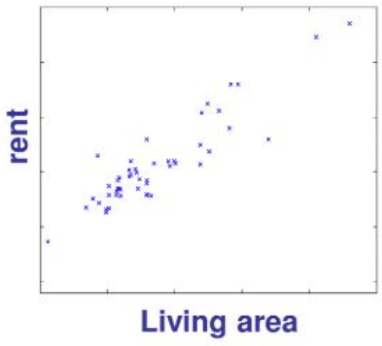
3. Select optimizer

Regression algorithms

Training Data $\{x^i, y^i\}_{i=1}^m$ → Learning Algorithm → Predictor $f: X \to Y$

$$y = \theta_0 + \theta_1 x_1 + \cdots + \theta_n x_n$$

- Features:
  - Living area, distance to campus, # of bedroom …
  - Denotes as $x = (x_1, x_2, \ldots, x_n)^\top$
- Target
  - Rent
  - Denote as y
- Training set
  - $X = (x^1, x^2, \ldots, x^m)$
  - $y = (y^1, y^2, \ldots, y^m)^\top$



Probabilistic Model:
Linear Regression Model with Gaussian Noise

- Assume y is a linear function of x (features) plus noise ϵ

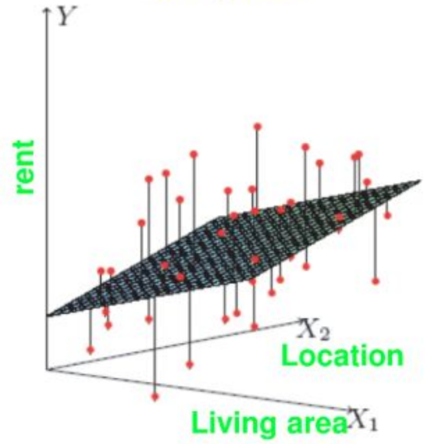
$$y = \theta_0 + \theta_1 x_1 + \cdots + \theta_n x_n + \epsilon$$

where ϵ is an error model as Gaussian $N(0, \sigma^2)$

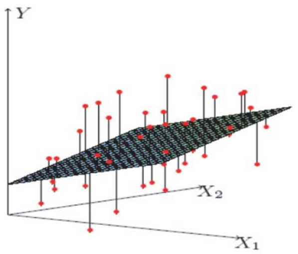
- Let $\theta = (\theta_0, \theta_1, \dots, \theta_n)^\top$, and augment data by one dimension

$$x \leftarrow (1, x)^\top$$

Then $y = \theta^\top x + \epsilon$



Probabilistic Model: Gaussian Likelihood

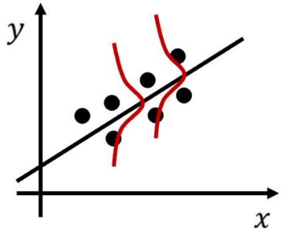


- Assume y is a linear in x plus noise ϵ

$$y = \theta^\top x + \epsilon$$

- Assume ϵ follows a Gaussian $N(0, \sigma)$

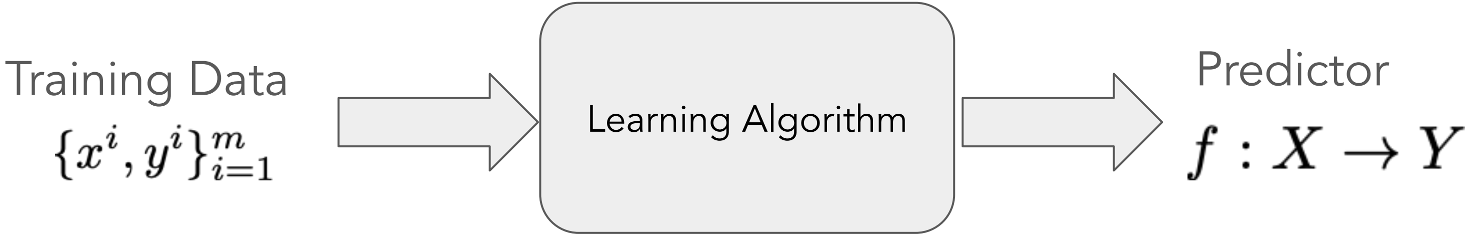
$$p(y^i \mid x^i; \theta) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\left(y^i - \theta^\top x^i\right)^2}{2\sigma^2}\right)$$



- By independence assumption, likelihood is

$$L(\theta) = \prod_i^m p(y^i \mid x^i; \theta) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^m \exp\left(-\frac{\sum_i^m \left(y^i - \theta^\top x^i\right)^2}{2\sigma^2}\right)$$

Regression algorithms



General ML Algorithm Pipeline

1. Build probabilistic models
2. Derive loss function (by MLE or MAP)
3. Select optimizer

Maximum log-Likelihood Estimation (MLE)

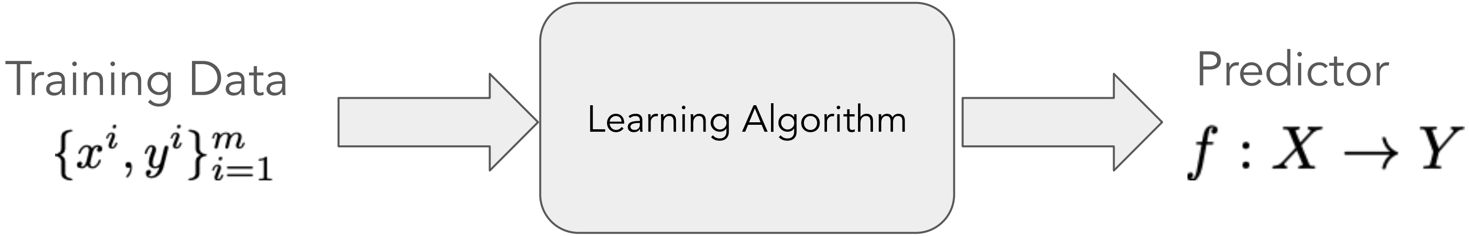
$$L(\theta) = \prod_{i}^{m} p\left(y^i \middle| x^i; \theta\right) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^m \exp\left(-\frac{\sum_i^m \left(y^i - \theta^\top x^i\right)^2}{2\sigma^2}\right)$$

Maximum log-Likelihood Estimation (MLE)

$$L(\theta) = \prod_{i}^{m} p(y^i | x^i; \theta) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^m \exp\left(-\frac{\sum_i^m \left(y^i - \theta^\top x^i\right)^2}{2\sigma^2}\right)$$

$$\max_{\theta} \ \log L(\theta) = -\frac{1}{2\sigma^2} \sum_{i=1}^{m} (y^i - \theta^\top x^i)^2 - m \log(\sqrt{2\pi}\sigma)$$

Regression algorithms



General ML Algorithm Pipeline

1. Build probabilistic models
2. Derive loss function (by MLE or MAP)
3. Select optimizer

Select Optimizer

$$\min_{\theta} \; -\log L(\theta) \propto \frac{1}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)^2$$

Select Optimizer

$$\min_{\theta} \; -\log L(\theta) \propto \frac{1}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)^2$$

- Necessary Condition
- (Stochastic) Gradient Descent

Necessary Condition

$$\min_{\theta} \; -\log L(\theta) \propto \frac{1}{m} \sum_{i=1}^{m} (y^i - \theta^\top x^i)^2$$

$$\frac{\partial \log L(\theta)}{\partial \theta} \qquad\qquad = 0$$

Necessary Condition

$$\min_{\theta} \; -\log L(\theta) \propto \frac{1}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)^2$$

$$\frac{\partial \log L(\theta)}{\partial \theta} = -\frac{2}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)x^{i\top} = 0$$

Necessary Condition

$$\min_{\theta} \; -\log L(\theta) \propto \frac{1}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)^2$$

$$\frac{\partial \log L(\theta)}{\partial \theta} = -\frac{2}{m}\sum_{i=1}^{m}\left(y^i - \theta^\top x^i\right)x^{i\top} = 0$$

$$\Leftrightarrow -\frac{2}{m}\sum_{i=1}^{m} y^i x^i + \frac{2}{m}\sum_{i=1}^{m} x^i x^{i\top}\theta = 0$$

Necessary Condition

$$\frac{\partial \log L(\theta)}{\partial \theta} = -\frac{2}{m}\sum_{i=1}^{m} y^i x^i + \frac{2}{m}\sum_{i=1}^{m} x^i {x^i}^{\top} \theta = 0$$

Necessary Condition

$$\frac{\partial \log L(\theta)}{\partial \theta} = -\frac{2}{m}\sum_{i=1}^{m} y^i x^i + \frac{2}{m}\sum_{i=1}^{m} x^i {x^i}^\top \theta = 0$$

$$\frac{\partial \log L(\theta)}{\partial \theta} = -\frac{2}{m}(x^1 \dots, x^m)(y^1 \dots, y^m)^\top + \frac{2}{m}(x^1, \dots x^m)(x^1, \dots x^m)^\top \theta = 0$$

Define $X = (x^1, x^2, \dots x^m), y = (y^1, y^2, \dots, y^m)^\top$, gradient becomes

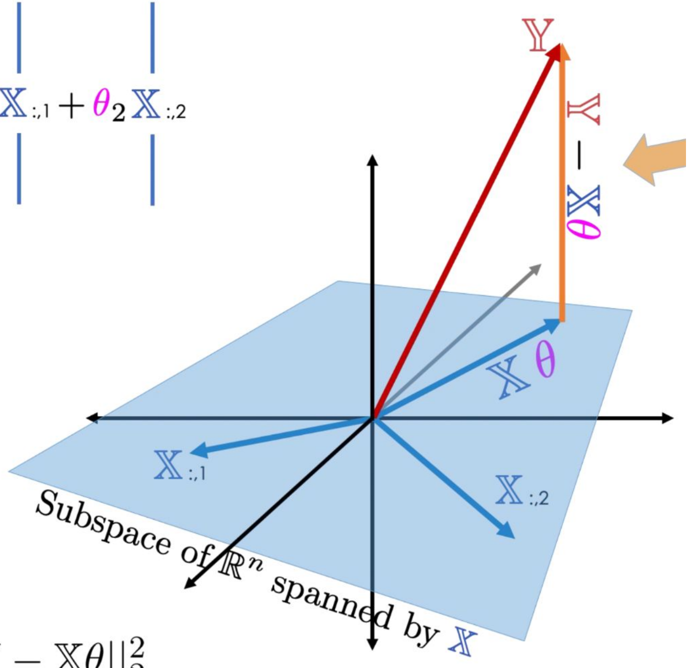
$$\frac{\partial \log L(\theta)}{\partial \theta} = -\frac{2}{m} Xy + \frac{2}{m} XX^\top \theta = 0$$

$$\Rightarrow \hat{\theta} = (XX^\top)^{-1} Xy$$

Geometric Interpretation

$$\hat{\theta} = (XX^{\top})^{-1}Xy$$

$$\underbrace{\begin{bmatrix} \hat{\mathbb{Y}} \end{bmatrix}}_{n \times 1} = \theta_1 \mathbb{X}_{:,1} + \theta_2 \mathbb{X}_{:,2}$$



$$R(\theta) = \frac{1}{n}||\mathbb{Y} - \mathbb{X}\theta||_2^2$$

Matrix Version of Necessary Condition

$$\min_{\theta} \; -\log L(\theta) \propto \frac{1}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)^2$$

$$= \frac{1}{m}(y - X^\top\theta)^\top(y - X^\top\theta)$$

$$\frac{\partial \log L(\theta)}{\partial \theta} =$$

Select Optimizer

$$\min_{\theta} \; -\log L(\theta) \propto \frac{1}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)^2$$

- Necessary Condition
- (Stochastic) Gradient Descent

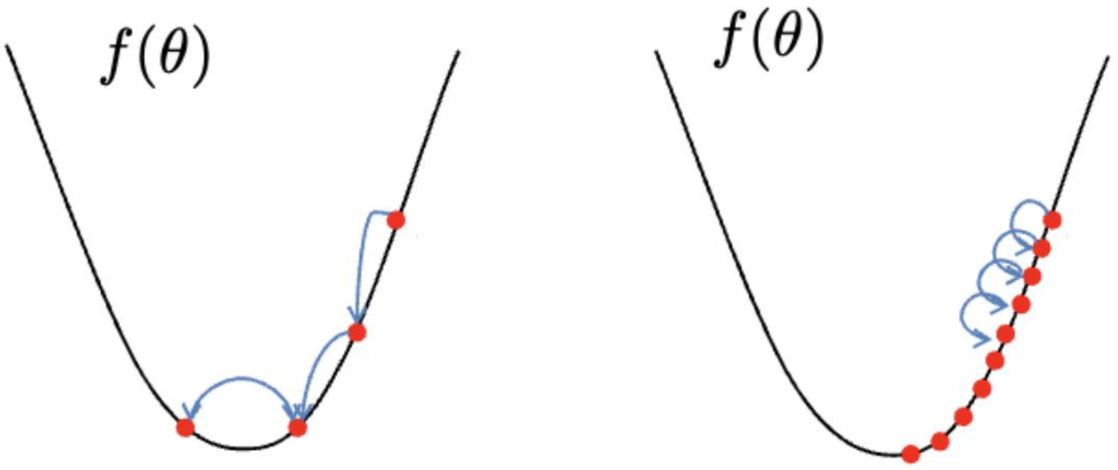
Gradient Method Revisit

$$\underbrace{\min_{\theta} \; -\log L(\theta) \propto \frac{1}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)^2}_{f(\theta)}$$

choose an initial $\theta^1 \in \mathbf{R}^d$ and $h^1 > 0$ (e.g., $\theta^1 = 0, h^1 = 1$)
for $k = 1,2,\ldots,k^{\max}$

1. compute $\nabla f(\theta^k)$; quit if $\|\nabla f(\theta^k)\|_2$ is small enough
2. form tentative update $\theta^{\text{tent}} = \theta^k - h^k \nabla f(\theta^k)$
3. if $f(\theta^{\text{tent}}) < f(\theta^k)$, set $\theta^{k+1} = \theta^{\text{tent}}, h^{k+1} = 1.2h^k$
4. else set $h^k := 0.5h^k$ and go to step 2

Effect of Learning Rate in GD



Large α ⇒ Fast convergence but larger residual error. Also possible oscillation.
Small α ⇒ Slow convergence but small residual error.

Gradient Calculation

$$\frac{\partial \log L(\theta)}{\partial \theta} = -\frac{2}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)x^i$$

form tentative update $\theta^{\text{tent}} = \theta^k - h^k \nabla f(\theta^k)$

$$\theta^k + \frac{h^k}{m}\sum_{i=1}^{m}(y^i - (\theta^k)^\top x^i)(x^i)^\top$$

Gradient Method Revisit

choose an initial $\theta^1 \in \mathbf{R}^d$ and $h^1 > 0$ (e.g., $\theta^1 = 0, h^1 = 1$)
for $k = 1,2, \dots, k^{\text{max}}$

Stochastic Approximation

1. compute $\nabla \cancel{f(\theta^k)}$; quit if $\|\nabla f(\theta^k)\|_2$ is small enough
2. form tentative update $\theta^{\text{tent}} = \theta^k - h^k \nabla f(\theta^k)$
3. if $f(\theta^{\text{tent}}) < f(\theta^k)$, set $\theta^{k+1} = \theta^{\text{tent}}, h^{k+1} = 1.2h^k$
4. else set $h^k := 0.5h^k$ and go to step 2

Stochastic Gradient Descent

$$\frac{\partial \log L(\theta)}{\partial \theta} = -\frac{2}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)x^i \approx \left(y^i - \hat{\theta}^{t^\top} x^i\right) x^i$$

Initialize $\theta^0 \in \mathbb{R}^d$ randomly Iterate until convergence:

1 Randomly sample a point (x_i, y_i) from the n data points

2 Compute noisy gradient $\tilde{g}^t = \left(y^i - (\theta^t)^\top x^i\right)\left(x^i\right)^\top$

3 Update (GD): $\theta^{t+1} = \theta^t - \eta \tilde{g}^t$

Recap

- Stochastic gradient update rule

$$\hat{\theta}^{t+1} \leftarrow \hat{\theta}^{t} + \beta \left(y^i - (\hat{\theta}^t)^\top x^i \right) x^i$$

  - Pros: online, low per-step cost
  - Cons: coordinate, (sometimes) slow-converging
- Gradient descent

$$\hat{\theta}^{t+1} \leftarrow \hat{\theta}^{t} + \frac{\alpha}{m} \sum_{i=1}^{m} \left(y^i - (\hat{\theta}^t)^\top x^i \right) x^i$$

  - Pros: fast-converging, easy to implement
  - Cons: need to read all data
- Solve normal equations

$$(X^\top X)\hat{\theta} = X^\top y$$

  - Pros: a single-shot algorithm! Easiest to implement
  - Cons: need to compute inverse, expensive, numerical issue (e.g., matrix is singular …)

Summary

General ML Algorithm Pipeline

1. Build probabilistic models
2. Derive loss function (by MLE or MAP)
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Polynomial Regression

Training Data

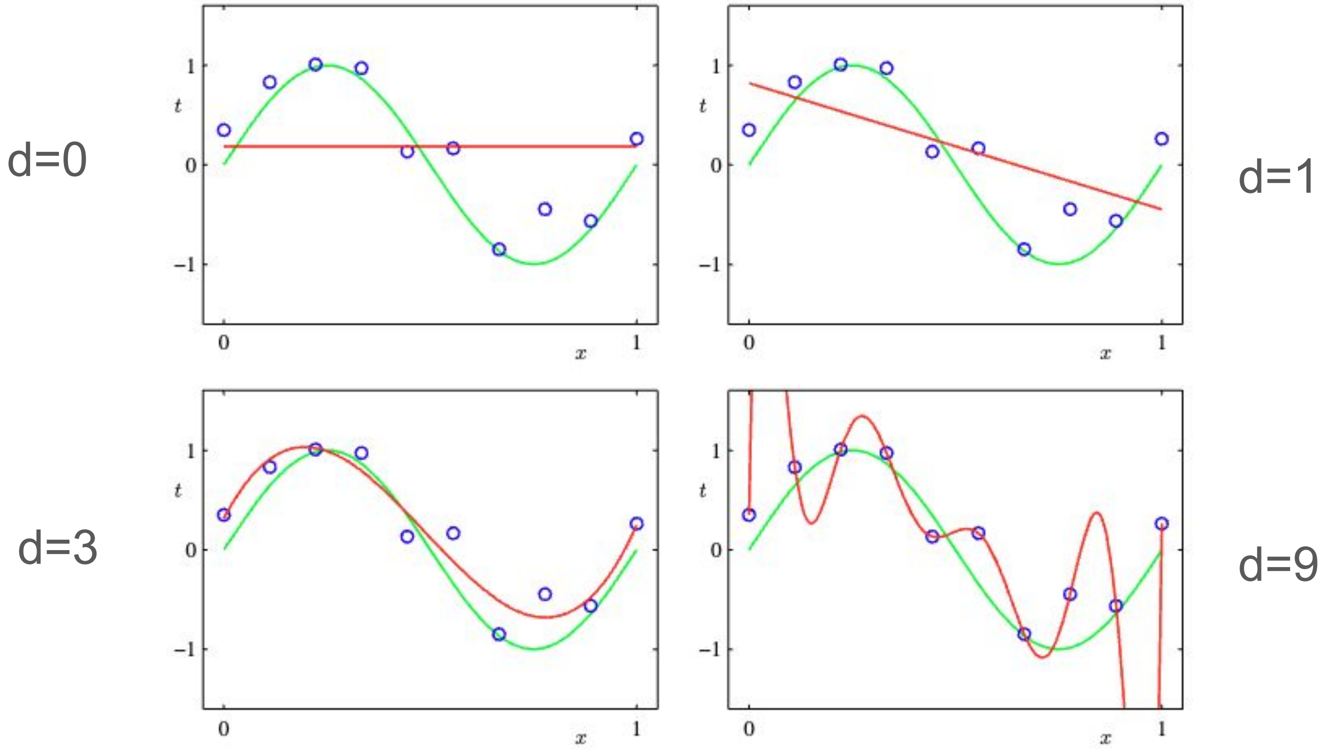
$\{\tilde{x}^i, y^i\}_{i=1}^m$ $\rightarrow$ Learning Algorithm $\rightarrow$ Predictor

$f : \tilde{X} \rightarrow Y$

- Features:
  - Living area, distance to campus, # of bedroom …
  - Denotes as $\tilde{x} = [1, x_1, (x_1)^2, \dots, (x_1)^d, \dots, x_n, \dots, (x_n)^d]$
- Target
  - Rent
  - Denote as y
- Training set
  - $\tilde{X} = [\tilde{x}^1, \tilde{x}^2, \dots, \tilde{x}^m]$
  - $y = (y^1, y^2, \dots, y^m)^\top$

$$\begin{aligned} y = \theta_0 &+ \theta_1^1 x_1 + \theta_1^2 (x_1)^2 + \theta_1^3 (x_1)^3 + \dots + \theta_1^d (x_1)^d \\ &+ \theta_2^1 x_2 + \theta_2^2 (x_2)^2 + \theta_2^3 (x_2)^3 + \dots + \theta_2^d (x_2)^d \\ &+ \dots \\ &+ \theta_n^1 x_n + \theta_n^2 (x_n)^2 + \theta_n^3 (x_n)^3 + \dots + \theta_n^d (x_n)^d \end{aligned}$$

Overfitting with Increased Degree



Summary

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Maximum a Posteriori (MAP)

$$L(\theta) = \prod_{i}^{m} p(y^i | x^i; \theta) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^m \exp\left(-\frac{\sum_i^m (y^i - \theta^\top x^i)^2}{2\sigma^2}\right)$$ Likelihood

$$p(\theta) \propto \exp(-\lambda \|\theta\|^2)$$ Gaussian Prior

Maximum a Posteriori (MAP)

$$L(\theta) = \prod_i^m p(y^i|x^i;\theta) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^m \exp\left(-\frac{\sum_i^m \left(y^i - \theta^\top x^i\right)^2}{2\sigma^2}\right)$$

Likelihood

$$p(\theta) \propto \exp(-\lambda\|\theta\|_2^2)$$

Gaussian Prior

$$p(\theta|\{x^i, y^i\}_{i=1}^m) = \frac{\prod_{i=1}^m p(y^i|x^i, \theta)p(\theta)}{\int \prod_{i=1}^m p(y^i|x^i, \theta)p(\theta)d\theta}$$

Posterior:
Bayes' Rule

Maximum a Posteriori (MAP)

$$L(\theta) = \prod_i^m p(y^i | x^i; \theta) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^m \exp\left(-\frac{\sum_i^m (y^i - \theta^\top x^i)^2}{2\sigma^2}\right)$$

Likelihood

$$p(\theta) \propto \exp(-\lambda \|\theta\|_2^2)$$

Gaussian Prior

$$p(\theta | \{x^i, y^i\}_{i=1}^m) = \frac{\prod_{i=1}^m p(y^i | x^i, \theta) p(\theta)}{\int \prod_{i=1}^m p(y^i | x^i, \theta) p(\theta) d\theta}$$

Posterior:
Bayes' Rule

$$\max_\theta \; \log p(\theta | \{x^i, y^i\}_{i=1}^m)$$

MAP

Maximum a Posteriori (MAP)

$$L(\theta) = \prod_{i}^{m} p\left(y^i | x^i; \theta\right) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^m \exp\left(-\frac{\sum_i^m \left(y^i - \theta^\top x^i\right)^2}{2\sigma^2}\right)$$

Likelihood

$$p(\theta) \propto \exp(-\lambda \|\theta\|_2^2)$$

Gaussian Prior

$$p(\theta | \{x^i, y^i\}_{i=1}^m) = \frac{\prod_{i=1}^m p(y^i | x^i, \theta) p(\theta)}{\int \prod_{i=1}^m p(y^i | x^i, \theta) p(\theta) d\theta}$$

Posterior:
Bayes' Rule

$$\max_\theta \; \log p(\theta | \{x^i, y^i\}_{i=1}^m) = \log L(\theta) + \log p(\theta)$$

$$\propto -\frac{1}{m} \sum_{i=1}^m (y^i - \theta^\top x^i)^2 - \lambda \|\theta\|_2^2$$

Ridge Regression

Maximum a Posteriori (MAP)

$$L(\theta) = \prod_i^m p(y^i|x^i;\theta) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^m \exp\left(-\frac{\sum_i^m (y^i - \theta^\top x^i)^2}{2\sigma^2}\right)$$ Likelihood

$$p(\theta) \propto \exp(-\lambda\|\theta\|_1)$$ Laplacian Prior

$$p(\theta|\{x^i, y^i\}_{i=1}^m) = \frac{\prod_{i=1}^m p(y^i|x^i, \theta)p(\theta)}{\int \prod_{i=1}^m p(y^i|x^i, \theta)p(\theta)d\theta}$$ Posterior: Bayes' Rule

$$\max_\theta \ \log p(\theta|\{x^i, y^i\}_{i=1}^m) = \log L(\theta) + \log p(\theta)$$ Lasso

$$\propto -\frac{1}{m}\sum_{i=1}^m (y^i - \theta^\top x^i)^2 - \lambda\|\theta\|_1$$

Select Optimizer

$$\min_{\theta} \; -\log p(\theta | \{x^i, y^i\}_{i=1}^m) \propto \frac{1}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)^2 + \lambda\|\theta\|_2^2$$

- Necessary Condition
- (Stochastic) Gradient Descent

Necessary Condition

$$\min_{\theta} \; -\log p(\theta | \{x^i, y^i\}_{i=1}^m) \propto \frac{1}{m} \sum_{i=1}^{m} (y^i - \theta^\top x^i)^2 + \lambda \|\theta\|_2^2$$

$$\frac{\partial \log L(\theta)}{\partial \theta} = -\frac{2}{m} \sum_{i=1}^{m} (y^i - \theta^\top x^i) x^i \qquad \frac{\partial \lambda \theta^\top \theta}{\partial \theta} = 2\lambda\theta$$

$$\frac{2}{m} \sum_{i=1}^{m} y^i x^i - \frac{2}{m} \sum_{i=1}^{m} x^i (x^i)^\top \theta + 2\lambda\theta = 0$$

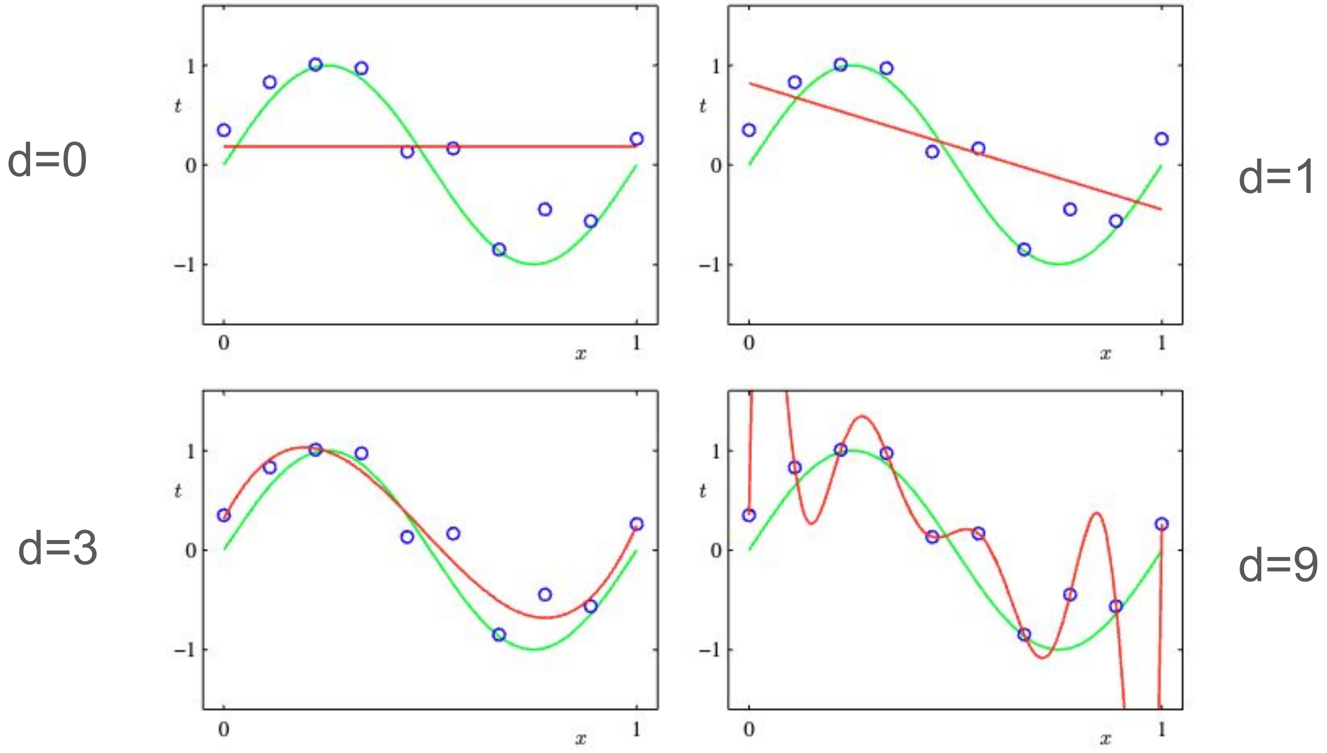
Necessary Condition

$$\frac{2}{m}\sum_{i=1}^{m} y^i x^i - \frac{2}{m}\sum_{i=1}^{m} x^i (x^i)^\top \theta + 2\lambda\theta = 0$$

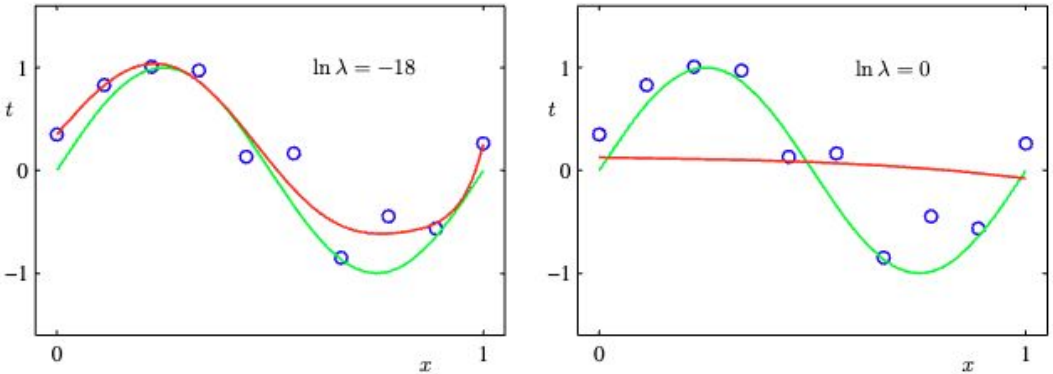
$$\frac{2}{m} X y - \frac{2}{m} X X^\top \theta + 2\lambda\theta = 0$$

$$\Rightarrow \hat{\theta} = (X X^\top + \lambda m I)^{-1} X y$$

Overfitting with Increased Degree



Best Degree?



$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
0.35	0.35	0.13
232.37	4.74	-0.05
-5321.83	-0.77	-0.06
48568.31	-31.97	-0.05
-231639.30	-3.89	-0.03
640042.26	55.28	-0.02
-1061800.52	41.32	-0.01
1042400.18	-45.95	-0.00
-557682.99	-91.53	0.00
125201.43	72.68	0.01

- MLE with appropriate d
- MAP with large d, regularization will select the appropriate model

MLE vs. MAP

MLE
- We chose the "best" θ that maximized the likelihood given data
- No prior

$$\hat{\theta} = (XX^\top)^{-1}Xy$$

- Numerical issue
- Overfitting

MAP
- We chose the "best" θ that maximized the posterior given data
- Prior matters

$$\hat{\theta} = (XX^\top + \lambda m I)^{-1}Xy$$

- No numerical issue
- Mitigate overfitting

Q&A