Generalized Linear Models

CS 229: Machine Learning
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(adapted from slides by Chris Ré; Emily Fox)

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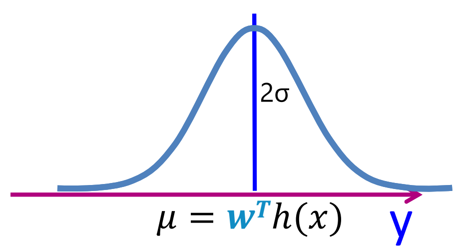
Models for data; how are these related?

- Linear regression with Gaussian errors

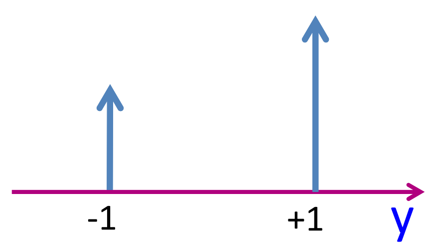
  $y_i = \boldsymbol{w}^{\boldsymbol{T}} h(x_i) + \ \varepsilon_i \ ; \ \varepsilon_i \sim N(0, \sigma^2)$

  ➔ $p(y|x, \boldsymbol{w}) = N(y; \boldsymbol{w}^{\boldsymbol{T}} h(x), \sigma^2)$



- Logistic regression

$$P(y = +1|x, w) = \frac{1}{1+\exp(-\boldsymbol{w}^{\boldsymbol{T}} h(x))}$$



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Background: Exponential Family Models

- **Rough motivation:** If P has a special form, then we can standardize (simplify) inference and learning

$$P(y;\eta) = b(y)\exp\left\{\eta^T T(y) - a(\eta)\right\}$$

- Here y , $a(\eta)$, and $b(y)$ are scalars. $T(y)$ is same dimension as the η.

These terms have names:

- η is called the natural parameter (also called canonical parameter)
- $T(y)$ is called the sufficient statistic.
- $b(y)$ is called the base measure, does not depend on η.
- $a(\eta)$ is called the log partition function, does not depend on y.

Example: Bernoulli $P(y;\phi) = \phi^y\,(1-\phi)^{1-y}$

- A Bernoulli random variable is an event (e.g., flipping a coin)
- How do we write this in exponential family form?

$$P(y;\eta) = b(y)\exp\left\{\eta^T T(y) - a(\eta)\right\} \quad e^{\log(\phi^y(1-\phi)^{1-y})}$$

- $\phi^y\,(1-\phi)^{1-y}$
$$= \exp\{y\log\phi + (1-y)\log(1-\phi)\}$$
$$= \exp\left\{y\log\frac{\phi}{1-\phi} + \log(1-\phi)\right\} \quad -\log(1+e)$$

- So $\quad \boxed{\eta = \log\frac{\phi}{1-\phi}}, T(y) = y, a(\eta) = -\log(1-\phi).$

Example: Gaussian, with fixed variance $\sigma^2 = 1$

$$P(y; \mu) = \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{1}{2}(y-\mu)^2\right\}.$$

- How do we write this in exponential family form?

$$P(y; \eta) = b(y) \exp\left\{\eta^T T(y) - a(\eta)\right\}$$

- Multiply out the square and group the terms

$$P(y; \mu) = \frac{1}{\sqrt{2\pi}} \exp\left\{-y^2/2\right\} \exp\left\{\mu y - \frac{1}{2}\mu^2\right\}.$$

- So

$$\eta = \mu,\ T(y) = y,\ a(\eta) = \frac{1}{2}\eta^2.$$

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The log partition function; $a(\eta)$ ensures normalization

$$P(y; \eta) = b(y) \exp\left\{\eta^T T(y) - a(\eta)\right\}$$

$$1 = \sum_y P(y; \eta) = e^{-a(\eta)} \sum_y b(y) \exp\left\{\eta^T T(y)\right\} = 1$$

$$\implies a(\eta) = \log \sum_y b(y) \exp\left\{\eta^T T(y)\right\}$$

Can compute all moments from gradients of $a(\eta)$; see notes Ch 3

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There are many canonical exponential family models!

$$P(y;\eta) = b(y)\exp\left\{\eta^T T(y) - a(\eta)\right\}$$

- Binary: Bernoulli
- Multiple classes: Multinomial (equiv. categorical)
- Real-valued: Gaussian
- Counts: Poisson
- Positive Reals: Gamma, Exponential
- Distributions: Dirichlet

For this course, we will generally use models where $T(y) = y$

Expectation for exponential family models

$$P(y;\eta) = b(y)\exp\left\{\eta^T T(y) - a(\eta)\right\}$$

- $E[T(y);\ \eta] = g(\eta)$; g is called the canonical response function
  - **NOTE:** g^{-1} is the canonical link function; notation varies (see class notes, Ch 3)

	Mean	response function g
Gaussian	μ	identity function
Bernoulli (assuming y in {0,1} instead of {-1,1} or some other set of values)	P(y=+1) (mean is different if y is not in {0,1})	sigmoid function (need slight modification if y is not in {0,1})

Generalized Linear Models (GLMs)
using Exponential Family Models

Recipe for Generalized linear Models

- Given input x and target y
- First: Pick a distribution based on y's type
  - Binary: Bernoulli
  - Multiple classes: Multinomial (equiv. categorical)
  - Real-valued: Gaussian
  - Counts: Poisson
  - Positive Reals: Gamma, Exponential
  - Distributions: Dirichlet

Recipe for Generalized Linear Models (GLMs)

Our model is linear in the natural parameters $\eta(x) = w^T h(x)$ and $T(y) = y$

- **Inference:** $\mu(x) = E[y|x; w] = g(w^T h(x))$ is the output
- **Learning:** $\max_w \log p(y|x; w)$, i.e., maximum likelihood
- **Algorithm:** (stochastic) gradient update (more on this later)

$$w^{\{t+1\}} = w^t + \alpha\left(y^i - \mu(x^i)\right)h(x^i)$$

Examples of GLMs

When $T(y) = y$, a generalized linear model has the property

$$E[y|x, \boldsymbol{w}] = g(\boldsymbol{w}^T h(x))$$

	Mean	Response function g
Linear regression	$\boldsymbol{w}^T h(x)$	identity function
Logistic regression (assuming y in {0,1} instead of {-1,1} or some other set of values)	$P(y = +1 \| x, \boldsymbol{w})$ (mean is different if y is not in {0,1})	sigmoid function (need slight modification if y is not in {0,1})

Similarly with multinomial, Poisson, gamma, exponential, …

Multiclass Classification
(aka softmax regression)

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Suppose we want to choose among k discrete values, e.g., {'Cat', 'Dog', 'Car', 'Bus'}, so $k = 4$

Encode as one-hot vectors, i.e., $y \in \{0,1\}^k$ and $\sum_j y_j = 1$

$P(y=i) = \theta^i$

$P(y) = \prod_{i=1}^{k} [\theta^i]^{1[y=i]}$

$$\begin{array}{cccc} \begin{pmatrix}1\\0\\0\\0\end{pmatrix} & \begin{pmatrix}0\\1\\0\\0\end{pmatrix} & \begin{pmatrix}0\\0\\1\\0\end{pmatrix} & \begin{pmatrix}0\\0\\0\\1\end{pmatrix} \\ \text{'Cat'} & \text{'Dog'} & \text{'Car'} & \text{'Bus'} \end{array}$$

A prediction is a distribution over k classes. We represent this using the SoftMax function (see notes Ch3 for derivation)

$$P(y=j|x;w) = \frac{\boxed{\exp(w_j^T h(x))}}{\sum_{i=1}^{k} \exp(w_i^T h(x))} \propto \theta^j$$

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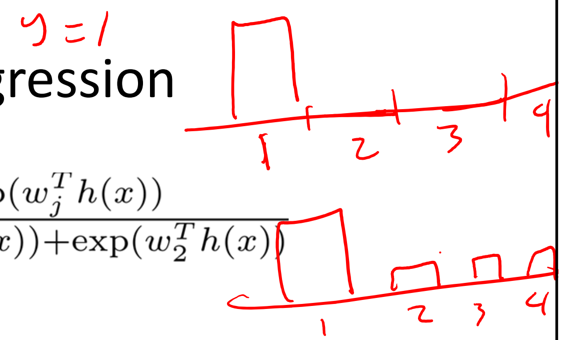
Compare k=2 to logistic regression



$$P(y = j|x; w) = \frac{\exp(w_j^T h(x))}{\exp(w_1^T h(x)) + \exp(w_2^T h(x))}$$

Hint, compare two class softmax regression vs. logistic regression using parameter $w_1 - w_2$

- **Note:** For general k, can write an equivalent model with k-1 classes (since probability must sum to 1)
- **Also note:** Multinomials are in the exponential family (see class notes Ch 3), can run everything learned so far!

Training multiclass classification (direct approach)

Let

$$\hat{p}_j = P(y = j|x; w) = \frac{\exp(w_j^T h(x))}{\sum_{i=1}^{k} \exp(w_i^T h(x))}$$

Maximize the probability of the given class! Popularly known as:

CROSSENTROPY$(p, \hat{p}) = \sum_j p(y = j|x) \log \hat{p}(y = j|x)$

p is the label (one hot vector), so this reduces to

$$-\log \hat{p}(y = i|x) = -\log \frac{\exp(w_i^T h(x))}{\sum_{j=1}^{k} \exp(w_j^T h(x))}$$

What you can do now…

- recognize exponential family models, and some of their properties
- recognize how exponential family models are related to generalized linear models
- recognize some special cases of exponential family models for regression, (binary, multiclass) classification, count regression
- inference and learning for generalized linear models
- familiar with SOFTMAX and CROSSENTROPY for multiclass classification

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Scaling up learning via SGD

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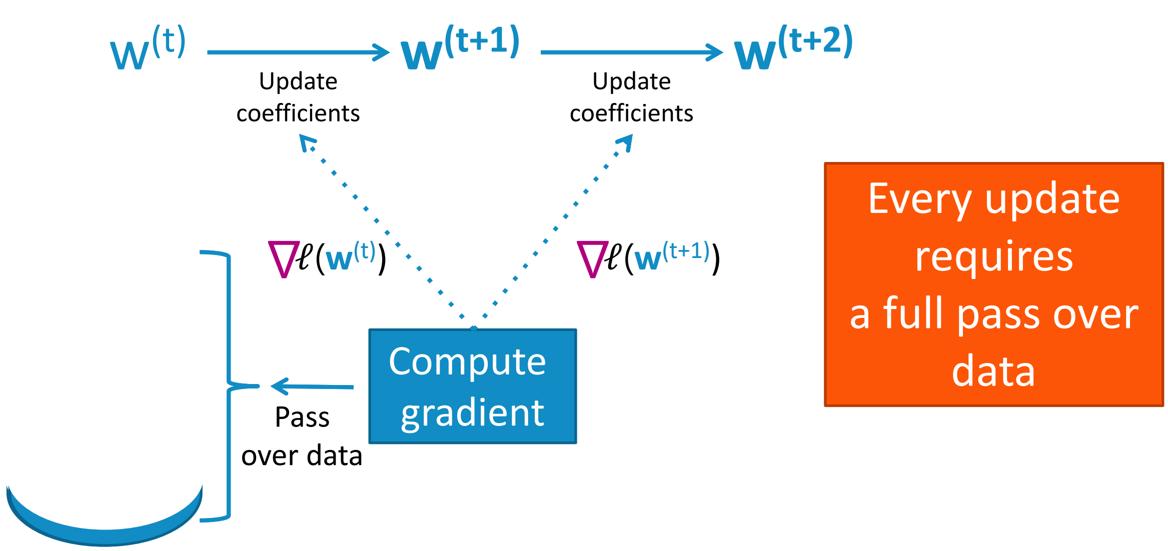
Stochastic gradient ascent/descent: Learning, one data point at a time

Why gradient ascent is slow…



More formally: How expensive is gradient ascent?

Sum over data points

$$\frac{\partial \ell(\mathbf{w})}{\partial \mathbf{w}_j} = \sum_{i=1}^{N} \underbrace{h_j(\mathbf{x}_i)\Big(\mathbb{1}[y_i = +1] - P(y = +1 \mid \mathbf{x}_i, \mathbf{w})\Big)}_{\text{Contribution of data point } x_i,y_i \text{ to gradient}}$$

Contribution of data point x_i,y_i to gradient

$$\frac{\partial \ell_i(\mathbf{w})}{\partial \mathbf{w}_j}$$

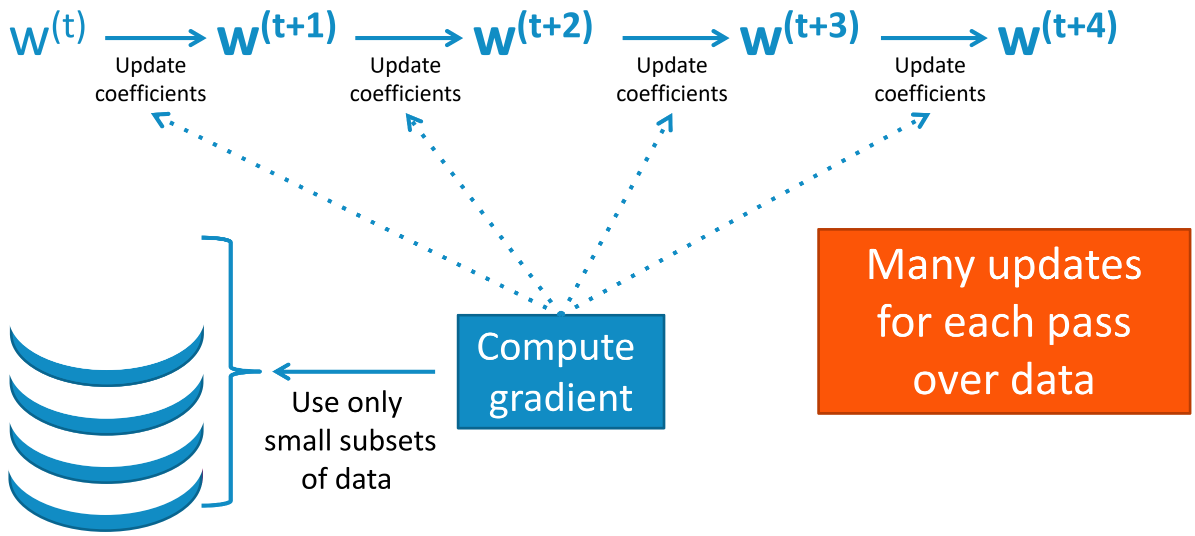
Every step requires touching every data point!!!

Sum over data points

$$\frac{\partial \ell(\mathbf{w})}{\partial \mathbf{w}_j} = \sum_{i=1}^{N} \frac{\partial \ell_i(\mathbf{w})}{\partial \mathbf{w}_j}$$

Time to compute contribution of $\mathbf{x}_i,\mathbf{y}_i$	# of data points (N)	Total time to compute 1 step of gradient ascent
1 millisecond	1000	1 sec
1 second	1000	16.7 mins
1 millisecond	10 million	2.8 hrs
1 millisecond	10 billion	115.7 days

Stochastic gradient ascent



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Example: Instead of all data points for gradient, use 1 data point only???

Sum over data points

Gradient ascent

$$\frac{\partial \ell(\mathbf{w})}{\partial \mathbf{w}_j} = \sum_{i=1}^{N} \frac{\partial \ell_i(\mathbf{w})}{\partial \mathbf{w}_j}$$

Stochastic gradient ascent

Each time, pick different data point i

$$\frac{\partial \ell(\mathbf{w})}{\partial \mathbf{w}_j} \approx \frac{\partial \ell_i(\mathbf{w})}{\partial \mathbf{w}_j}$$

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Stochastic gradient ascent for logistic regression

init $w^{(1)}$=0, t=1

until converged

for i=1,...,N

for j=0,...,D

Sum over data points

Each time, pick different data point i

partial[j] = $\cancel{\sum_{i=1}^{N}} h_j(\mathbf{x}_i)\Big(\mathbb{1}[y_i = +1] - P(y = +1 \mid \mathbf{x}_i, \mathbf{w}^{(t)})\Big)$

$w_j^{(t+1)} \leftarrow w_j^{(t)} + \eta$ partial[j]

t ← t + 1

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Stochastic gradient for L2-regularized objective

Total derivative = $\sum_{i=1}^{N} \frac{\partial \ell_i(\mathbf{w})}{\partial \mathbf{w}_j} - 2\,\lambda\, w_j$ $\boxed{\text{partial[j]}}$

What about regularization term?

Each time, pick different data point i

Stochastic gradient ascent

Total derivative $\approx \frac{\partial \ell_i(\mathbf{w})}{\partial \mathbf{w}_j} - \frac{2}{N}\,\lambda\, w_j$ $\boxed{\text{partial[j]}}$

Each data point contributes 1/N to regularization

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Comparing computational time per step

Gradient ascent

$$\frac{\partial \ell(\mathbf{w})}{\partial \mathbf{w}_j} = \sum_{i=1}^{N} \frac{\partial \ell_i(\mathbf{w})}{\partial \mathbf{w}_j}$$

Stochastic gradient ascent

$$\frac{\partial \ell(\mathbf{w})}{\partial \mathbf{w}_j} \approx \frac{\partial \ell_i(\mathbf{w})}{\partial \mathbf{w}_j}$$

Time to compute contribution of $\mathbf{x}_i,\mathbf{y}_i$	# of data points (N)	Total time for 1 step of gradient	Total time for 1 step of stochastic gradient
1 millisecond	1000	1 second	1 ms
1 second	1000	16.7 minutes	1 s
1 millisecond	10 million	2.8 hours	1 ms
1 millisecond	10 billion	115.7 days	1 ms

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Which one is better??? Depends…

Algorithm	Time per iteration	Total time to convergence for large data: In theory	Total time to convergence for large data: In practice	Sensitivity to parameters
Gradient	Slow for large data	Slower	Often slower	Moderate
Stochastic gradient	Always fast	Faster	Often faster	Very high

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Summary of stochastic gradient

- Tiny change to gradient ascent
- Much better scalability
- Huge impact in real-world
- Very tricky to get right in practice

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Why would stochastic gradient ever work???

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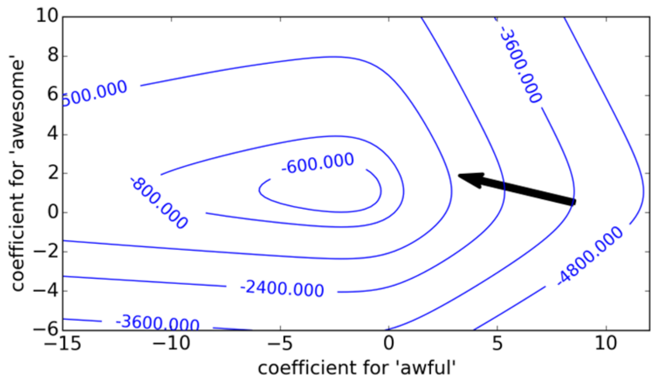
Gradient is direction of steepest ascent



Gradient is "best" direction, but
any direction that goes "up" would be useful

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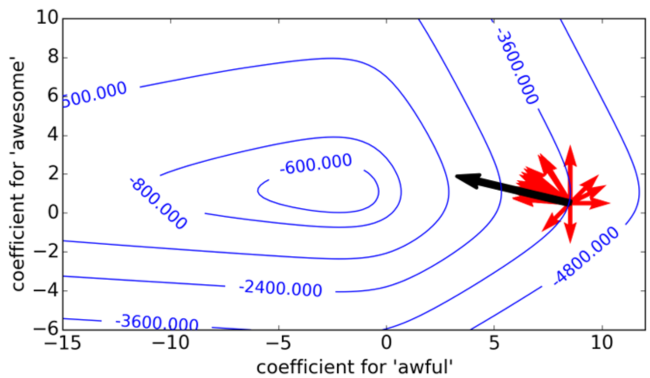
In ML, steepest direction is sum of "little directions" from each data point



Sum over
data points

$$\frac{\partial \ell(\mathbf{w})}{\partial \mathbf{w}_j} = \sum_{i=1}^{N} \frac{\partial \ell_i(\mathbf{w})}{\partial \mathbf{w}_j}$$

For most data points,
contribution points "up"

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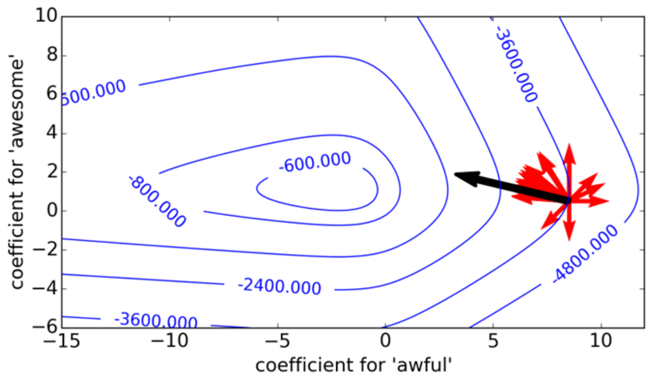
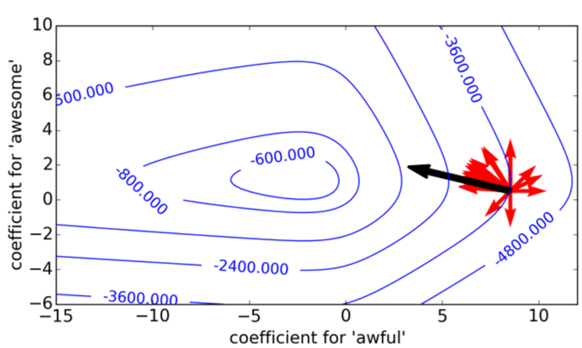
Stochastic gradient:
Pick a data point and move in direction



$$\frac{\partial \ell(\mathbf{w})}{\partial \mathbf{w}_j} \approx \frac{\partial \ell_i(\mathbf{w})}{\partial \mathbf{w}_j}$$

Most of the time, total likelihood will increase

Stochastic gradient ascent:
Most iterations increase likelihood, but sometimes decrease it ➔
On average, make progress



until converged

  for i=1,…,N

    for j=0,…,D

      $w_j^{(t+1)} \leftarrow w_j^{(t)} + \eta \dfrac{\partial \ell_i(\mathbf{w})}{\partial \mathbf{w}_j}$

    $t \leftarrow t + 1$

Convergence path

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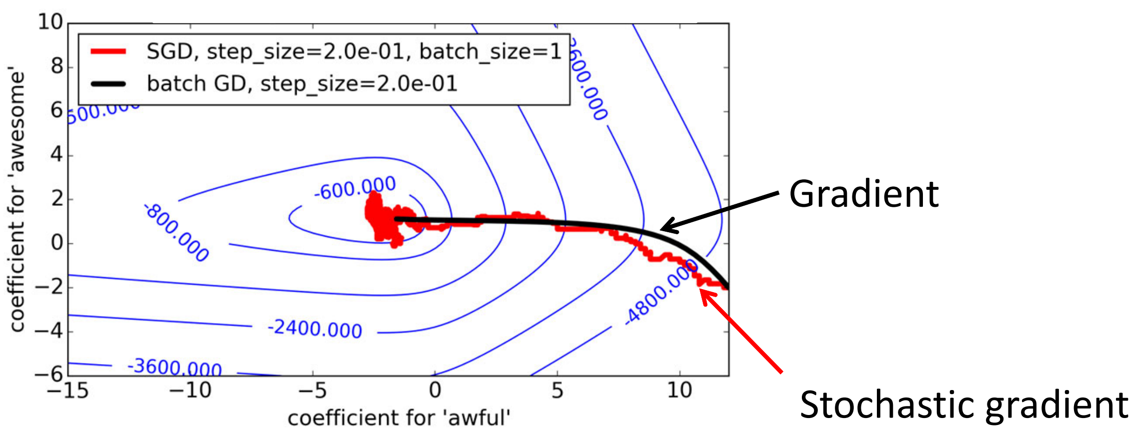
Convergence paths



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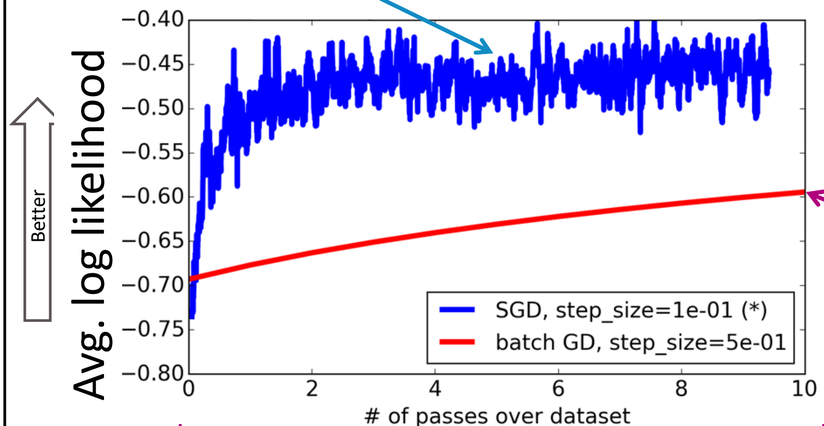
Stochastic gradient convergence is "noisy"

Stochastic gradient makes "noisy" progress

Stochastic gradient achieves higher likelihood sooner, but it's noisier



Gradient usually increases likelihood smoothly

Total time proportional to # passes over data

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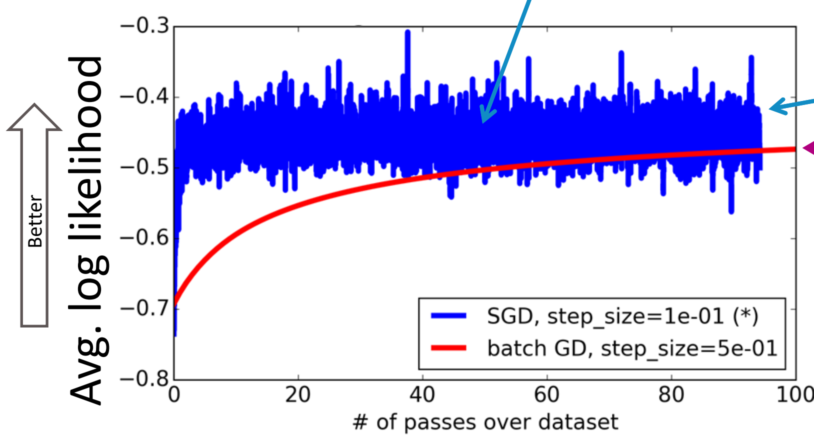
Eventually, gradient catches up

Note: should only trust "average" quality of stochastic gradient



Stochastic gradient

Gradient

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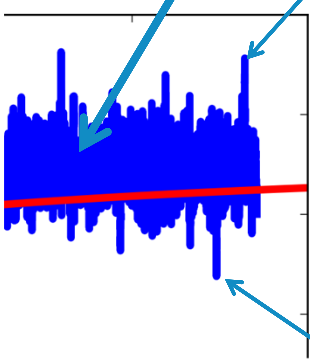
The last coefficients may be really good or really bad!! ☹

Stochastic gradient will eventually oscillate around a solution

$w^{(1005)}$ was good



$w^{(1000)}$ was bad

How do we minimize risk of picking bad coefficients

Minimize noise: don't return last learned coefficients

Output average:

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

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Summary of why stochastic gradient works

- Gradient finds direction of steeps ascent
- Gradient is sum of contributions from each data point
- Stochastic gradient uses direction from 1 data point
- On average increases likelihood, sometimes decreases
- Stochastic gradient has "noisy" convergence

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Online learning:
Fitting models from streaming data

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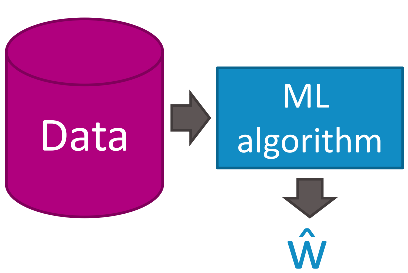
Batch vs online learning

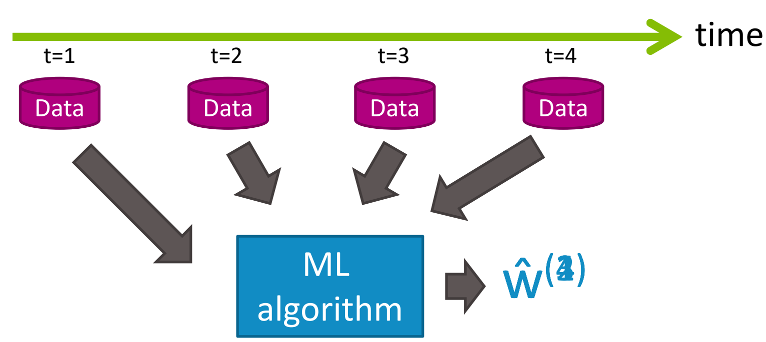
Batch learning

- All data is available at start of training time



Online learning

- Data arrives (streams in) over time
  - Must train model as data arrives!



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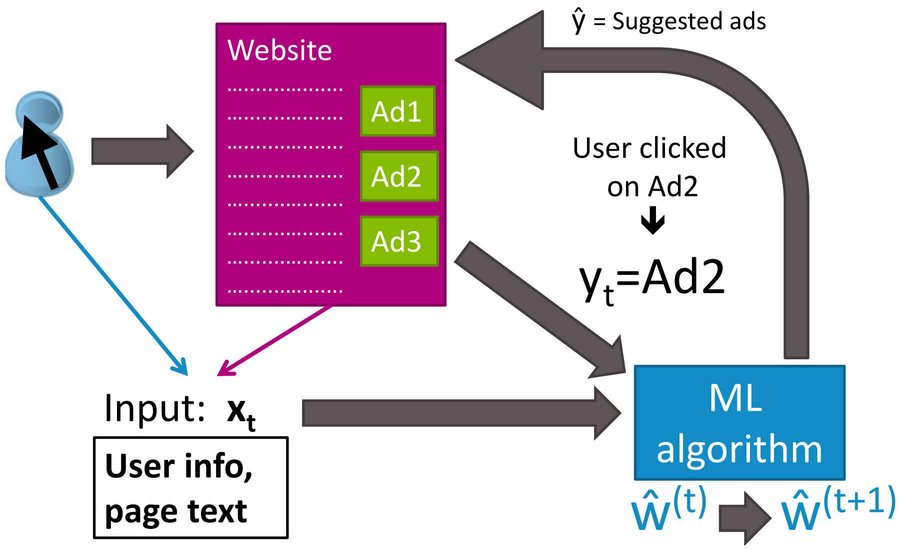
Online learning example: Ad targeting



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Online learning problem

- Data arrives over each time step t:
  - Observe input x_t
    - Info of user, text of webpage
  - Make a prediction $\hat{y}_t$
    - Which ad to show
  - Observe true output y_t
    - Which ad user clicked on

Need ML algorithm to update coefficients each time step!

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Stochastic gradient ascent can be used for online learning!!!

- init $w^{(1)}$=0, t=1
- Each time step t:
  - Observe input x_t
  - Make a prediction $\hat{y}_t$
  - Observe true output y_t
  - Update coefficients:

for j=0,…,D

$$w_j^{(t+1)} \leftarrow w_j^{(t)} + \eta \frac{\partial \ell_t(\mathbf{w})}{\partial \mathbf{w}_j}$$

Summary of online learning

Data arrives over time

Must make a prediction every time new data point arrives

Observe true class after prediction made

Want to update parameters immediately

Summary of stochastic gradient descent

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What you can do now…

- Significantly speedup learning algorithm using stochastic gradient
- Describe intuition behind why stochastic gradient works
- Apply stochastic gradient in practice
- Describe online learning problems
- Relate stochastic gradient to online learning

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Stochastic gradient descent more formally

OPTIONAL

Learning Problems as Expectations

- Minimizing loss in training data:
  - Given dataset:
    - Sampled iid from some distribution p(**x**) on features:
  - Loss function, e.g., hinge loss, logistic loss,…
  - We often minimize loss in training data:

$$\ell_{\mathcal{D}}(\mathbf{w}) = \frac{1}{N}\sum_{j=1}^{N}\ell(\mathbf{w},\mathbf{x}^j)$$

- However, we should really minimize expected loss on all data:

$$\ell(\mathbf{w}) = E_{\mathbf{x}}\left[\ell(\mathbf{w},\mathbf{x})\right] = \int p(\mathbf{x})\ell(\mathbf{w},\mathbf{x})d\mathbf{x}$$

- So, we are approximating the integral by the average on the training data

Gradient Ascent in Terms of Expectations

- "True" objective function:

$$\ell(\mathbf{w}) = E_{\mathbf{x}}\left[\ell(\mathbf{w},\mathbf{x})\right] = \int p(\mathbf{x})\ell(\mathbf{w},\mathbf{x})d\mathbf{x}$$

- Taking the gradient:
- "True" gradient ascent rule:
- How do we estimate expected gradient?

SGD: Stochastic Gradient Ascent (or Descent)

- "True" gradient: $\nabla\ell(\mathbf{w}) = E_{\mathbf{x}}\left[\nabla\ell(\mathbf{w},\mathbf{x})\right]$
- Sample based approximation:
- What if we estimate gradient with just one sample???
  - Unbiased estimate of gradient
  - Very noisy!
  - Called stochastic gradient ascent (or descent)
    - Among many other names
  - VERY useful in practice!!!

