# More categorical variables and Monte Carlo CPSC 440/550: Advanced Machine Learning cs.ubc.ca/~dsuth/440/23w2 <br> University of British Columbia, on unceded Musqueam land 

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\text { 2023-24 Winter Term } 2 \text { (Jan-Apr 2024) }
$$

## Outline

(1) Monte Carlo
(2) Categorical MLE, MAP
(3) Multi-class classification

## Motivation: probabilistic inference

- Given a general model, we often want to make inferences
- Marginals: what's the probability that $X_{i}=c$ ?
- Conditionals: what's the probability that $X_{i}=c$, given that $X_{i^{\prime}}=c^{\prime}$ ?
- This has been simple for the models we've seen so far
- For Bernoulli/categorical, computing probabilities is straightforward
- For product of Bernoullis (or categoricals), assumed everything is independent
- For many models, inference has no closed form or might be NP-hard
- In these cases, we'll often use Monte Carlo approximations


## Monte Carlo: marginalization by sampling

- A basic Monte Carlo method for estimating probabilities of events:
- Step 1: Generate a lot of samples $x^{(i)}$ from our model

$$
X=\left[\begin{array}{llll}
0 & 0 & 1 & 0 \\
1 & 1 & 1 & 0 \\
0 & 1 & 1 & 1 \\
1 & 1 & 1 & 1
\end{array}\right]
$$

- Step 2: Count how often the event occurred in the samples

$$
\operatorname{Pr}\left(X_{2}=1\right) \approx \frac{3}{4} \quad \operatorname{Pr}\left(X_{3}=0\right) \approx 0
$$

- This very simple idea is one of the most important algorithms in ML/statistics
- Modern versions developed to build better nuclear weapons :/
- "Sample" from a physics simulator, see how often it leads to a chain reaction


## Monte Carlo to approximate probabilities

- Monte Carlo estimate of the probability of an event $A$ :

$$
\frac{\text { number of samples where } A \text { happened }}{\text { number of samples }}=\frac{1}{n} \sum_{i=1}^{n} \mathbb{1}\left(A \text { happened in } x^{(i)}\right)
$$

- You can think of this as the MLE of a binary variable $\mathbb{1}$ ( $A$ happened)
- Approximating probability of a pair of independent dice adding to 7:
- Roll two dice, check if they add to 7
- Roll two dice, check if they add to 7
- Roll two dice, check if they add to 7
- Roll two dice, check if they add to 7
- Roll two dice, check if they add to 7
- Roll two dice, check if they add to 7
- ...
- Monte Carlo estimate: fraction where they add to 7


## Monte Carlo to approximate probabilities

- Recall the problem of modeling (Lib, CPC, NDP, GRN, PPC)
- From 100 samples, what's the probability that $n_{\text {Lib }}>\max \left(n_{\mathrm{CPC}}, n_{\mathrm{NDP}}, \ldots\right)$ ?
- Can answer this in closed form with math ... or think less and do Monte Carlo
- Generate 100 samples, check who won
- Generate 100 samples, check who won
- Approximate probability by fraction of times they won
- Another example: probability that $\operatorname{Beta}(\alpha, \beta)$ is above 0.7


## Monte Carlo to estimate the mean

- A Monte Carlo estimate for the mean: the mean of the samples

$$
\mathbb{E}[X] \approx \frac{1}{n} \sum_{i=1}^{n} x^{(i)}
$$

- A Monte Carlo approximation of the expected value of $X^{2}$ :

$$
\mathbb{E}\left[X^{2}\right] \approx \frac{1}{n} \sum_{i=1}^{n}\left(x^{(i)}\right)^{2}
$$

- A Monte Carlo approximation of the expected value of $g(X)$ :

$$
\mathbb{E}[g(X)] \approx \frac{1}{n} \sum_{i=1}^{n} g\left(x^{(i)}\right) \quad \mathbb{E}[g(X)]=\sum_{x \in \mathcal{X}} p(x) g(x) \text { or } \int_{x \in \mathcal{X}} p(x) g(x) \mathrm{d} x
$$

- Most general form: $g(x)=x, g(x)=x^{2}, g(x)=\mathbb{1}(A$ happens on $x)$

$$
\mathbb{E}[\mathbb{1}(A \text { happens on } x)]=\int_{x \in \mathcal{X}} p(x) \mathbb{1}(A \text { happens on } x) \mathrm{d} x=\int_{x: A \text { happens }} p(x) \mathrm{d} x=\operatorname{Pr}(A)
$$

## Monte Carlo: theory

- Let $\mu=\mathbb{E}[g(X)]$ be the value we want to compute, $\hat{\mu}$ our estimate
- Assume $\sigma^{2}=\operatorname{Var}[g(X)]$ exists and is bounded ("not infinite")
- With iid samples, Monte Carlo gives an unbiased estimate of $\mu$
- Expected value of $\hat{\mu}$, over samples we might draw, is exactly $\mu$
- Monte Carlo estimate "converges to $\mu$ " as $n \rightarrow \infty$
- Estimate gets arbitrarily close to $\mu$ as $n$ increases: (strong) law of large numbers
- Expected squared error is exactly $\mathbb{E}(\hat{\mu}-\mu)^{2}=\frac{\sigma^{2}}{n}$
- $\hat{\mu}$ is approximately normal with mean $\mu$ and variance $\frac{\sigma^{2}}{n}$ (central limit theorem)


## Example application: Snakes and Ladders



- Kid's game "Snakes and Ladders":
- Start at 1 , roll die, move the marker, follow snake/ladder
- Absolutely no decision-making: can simulate the game
- How long does this game go for?
- Run the game lots of times, see how many turns it took

| 100 | 89 | 9 | 97 | \% | \% | \% | \% | 92 | 9 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 31. | 82 | \& | 84 | 85 | O | 4 | 88 | 89 | (30) |
| 89 | 79 | 78 | 77 | ${ }^{6}$ | 78 | $74)$ | 7s | 72 | 40 |
| 61 |  |  | m |  |  |  | s | 69 | 70 |
| 69 |  |  | 57 |  |  | 54 | 53 | 52 | 31 |
| 41 |  |  | 4 |  | 45 | 47 | * | F | 50 |
| 40 | 39 |  | 37 |  | 35 |  | ${ }^{33}$ | 32 | 31 |
| 28. |  |  |  | $25$ | 20 | 27 | 2 t |  | 36 |
| 20 |  |  | 17 | $\%$ | 15 | 24 | 13 | 12. | 1 |
| 率 | 2 | 3 |  |  |  | 7 | 8 | 6/ | 10 |




## Conditional probabilities with Monte Carlo

- "How much loooonger will this game go?"
- Just simulate starting from current game state
- "What's the probability the game will go >100 turns, if it's already gone 50?"
- One approach:

$$
\operatorname{Pr}(A \mid B)=\frac{\operatorname{Pr}(A \cap B)}{\operatorname{Pr}(B)} \approx \frac{\frac{1}{n} \sum_{i=1}^{n} \mathbb{1}\left(A \text { and } B \text { happened on } x^{(i)}\right)}{\frac{1}{n} \sum_{i=1}^{n} \mathbb{1}\left(B \text { happened on } x^{(i)}\right)}
$$

- This is one instance of rejection sampling (more later)
- If $B$ is rare, most samples are wasted


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## MLE for categorical distribution

- How do we learn a categorical model?

$$
\mathbf{X}=\left[\begin{array}{c}
\text { NDP } \\
\mathrm{Lib} \\
\mathrm{Lib} \\
\mathrm{CPC} \\
\vdots
\end{array}\right] \xrightarrow{\text { density estimator }} \quad \boldsymbol{\theta}=\left[\begin{array}{l}
\operatorname{Pr}(X=\mathrm{Lib})=0.404 \\
\operatorname{Pr}(X=\mathrm{NDP})=0.307 \\
\operatorname{Pr}(X=\mathrm{CPC})=0.216 \\
\operatorname{Pr}(X=\mathrm{Grn})=0.039 \\
\operatorname{Pr}(X=\mathrm{PPC})=0.032
\end{array}\right]
$$

- Like before, start with maximum likelihood estimation (MLE):

$$
\hat{\boldsymbol{\theta}} \in \underset{\theta}{\arg \max } p(\mathbf{X} \mid \boldsymbol{\theta})
$$

- Like before, MLE will be $\theta_{c}=\frac{n_{c}}{n}$ (the portion of $c s$ in the data)
- Like before, derivation is more complicated than the result


## Derivation of the MLE that doesn't work

- We showed last time that the likelihood is

$$
p(\mathbf{X} \mid \boldsymbol{\theta})=\theta_{1}^{n_{1}} \cdots \theta_{k}^{n_{k}}
$$

- So, the log-likelihood is

$$
\log p(\mathbf{X} \mid \boldsymbol{\theta})=n_{1} \log \theta_{1}+\cdots+n_{k} \log \theta_{k}
$$

- Take the derivative for a particular $\theta_{c}$ :

$$
\frac{\partial}{\partial \theta_{c}} \log p(\mathbf{X} \mid \boldsymbol{\theta})=\frac{n_{c}}{\theta_{c}}
$$

- Set the derivative to zero:

$$
\frac{n_{c}}{\theta_{c}}=0
$$

- ... huh?


## Fixing the derivation

- Setting the derivative to zero doesn't work
- Ignores the constraint that $\sum_{c} \theta_{c}=1$
- Some ways to enforce constraints (see e.g. this StackExchange thread):
- Use "Lagrange multipliers," find stationary point of the "Lagrangian"
- Define $\theta_{k}=1-\sum_{c=1}^{k-1} \theta_{c}$, replace in the objective function
- We'll take a different way:
- Use a different parameterization $\tilde{\theta}_{c}$ that doesn't have this constraint
- Compute the MLE for the $\tilde{\theta}_{c}$ by setting derivative to zero
- Convert from the $\tilde{\theta}_{c}$ to $\theta_{c}$


## Unnormalized parameterization

- Let's have $\tilde{\theta}_{c}$ be unnormalized:

$$
\operatorname{Pr}\left(X=c \mid \tilde{\theta}_{1}, \ldots, \tilde{\theta}_{k}\right) \propto \tilde{\theta}_{c}
$$

- Still need each $\tilde{\theta}_{c} \geq 0$
- Can then find

$$
p(c \mid \tilde{\boldsymbol{\theta}})=\frac{\tilde{\theta}_{c}}{\sum_{i=1}^{k} \tilde{\theta}_{c}}=\frac{\tilde{\theta}_{c}}{Z_{\tilde{\boldsymbol{\theta}}}}
$$

- The "normalizing constant" $Z_{\tilde{\theta}}$ makes the total probability 1
- Don't need the explicit sum-to- 1 constraint anymore
- Note: constant for different $x$; not constant for different $\boldsymbol{\theta}$
- To convert from unnormalized to normalized: $\theta_{c}=\tilde{\theta}_{c} / Z_{\tilde{\boldsymbol{\theta}}}$


## Derivation of the MLE that does work

- The likelihood in terms of the unnormalized parameters is

$$
p(\mathbf{X} \mid \tilde{\boldsymbol{\theta}})=\left(\frac{\tilde{\theta}_{1}}{Z_{\tilde{\boldsymbol{\theta}}}}\right)^{n_{1}} \cdots\left(\frac{\tilde{\theta}_{k}}{Z_{\tilde{\boldsymbol{\theta}}}}\right)^{n_{k}}=\frac{1}{Z_{\tilde{\boldsymbol{\theta}}}^{n}} \tilde{\theta}_{1}^{n_{1}} \cdots \tilde{\theta}_{k}^{n_{k}}
$$

- So, the log-likelihood is

$$
\log p(\mathbf{X} \mid \tilde{\boldsymbol{\theta}})=n_{1} \log \tilde{\theta}_{1}+\cdots+n_{k} \log \tilde{\theta}_{k}-n \log Z_{\tilde{\boldsymbol{\theta}}}
$$

- Take the derivative for a particular $\tilde{\theta}_{c}$ :

$$
\frac{\partial}{\partial \tilde{\theta}_{c}} \log p(\mathbf{X} \mid \tilde{\boldsymbol{\theta}})=\frac{n_{c}}{\tilde{\theta}_{c}}-\frac{n}{Z_{\tilde{\boldsymbol{\theta}}}} \frac{\partial Z_{\tilde{\boldsymbol{\theta}}}}{\partial \tilde{\boldsymbol{\theta}}_{c}}=\frac{n_{c}}{\tilde{\theta}_{c}}-\frac{n}{Z_{\tilde{\boldsymbol{\theta}}}} \quad \text { since } \frac{\partial}{\partial \tilde{\theta}_{c}}\left(\tilde{\theta}_{1}+\cdots+\tilde{\theta}_{k}\right)=1
$$

- Set the derivative to zero:

$$
\frac{n_{c}}{\tilde{\theta}_{c}}=\frac{n}{Z_{\tilde{\boldsymbol{\theta}}}} \quad \text { so } \quad \frac{\tilde{\theta}_{c}}{Z_{\tilde{\boldsymbol{\theta}}}}=\frac{n_{c}}{n}
$$

- Can check this objective is concave, so this is a max
- Many solutions, but all the same after normalizing


## MAP estimate, Dirichlet prior

- As before, might prefer MAP estimate over MLE
- Often becomes more important for large $k$ : lots of parameters!
- Most common prior is the Dirichlet distribution:

$$
p\left(\theta_{1}, \ldots, \theta_{k} \mid \alpha_{1}, \ldots, \alpha_{k}\right) \propto \theta_{1}^{\alpha_{1}-1} \cdots \theta_{k}^{\alpha_{k}-1}
$$

- Generalization of the beta distribution to $k$ classes
- Requires each $\alpha_{c}>0$
- This is a distribution over $\theta$
- Probability distribution over possible (categorical) probability distributions


## Dirichlet distribution

- Wikipedia's visualizations for $k=3$ :

https://en.wikipedia.org/wiki/Dirichlet_distribution


## MAP estimate for Dirichlet-Categorical

- Reason to use the Dirichlet: again because posterior is simple

$$
\begin{aligned}
p(\boldsymbol{\theta} \mid \mathbf{X}, \boldsymbol{\alpha}) \propto p(\mathbf{X} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta} \mid \boldsymbol{\alpha}) & \propto \theta_{1}^{n_{1}} \cdots \theta_{k}^{n_{k}} \theta_{1}^{\alpha_{1}-1} \cdots \theta_{k}^{\alpha_{k}-1} \\
& =\theta_{1}^{\left(n_{1}+\alpha_{1}\right)-1} \cdots \theta_{k}^{\left(n_{k}+\alpha_{k}\right)-1}
\end{aligned}
$$

i.e. it's Dirichlet again with parameters $\tilde{\alpha}_{c}=n_{c}+\alpha_{c}$

- A few more steps show MAP for a categorical with Dirichlet prior is

$$
\hat{\theta}_{c}=\frac{n_{c}+\alpha_{c}-1}{\sum_{c^{\prime}=1}^{k}\left(n_{c^{\prime}}+\alpha_{c^{\prime}}-1\right)}
$$

- Dirichlet has $k$ hyper-parameters $\alpha_{c}$
- Often use $\alpha_{c}=\alpha$ for some $\alpha \in \mathbb{R}$ : one hyperparameter
- Makes the MLE $\hat{\theta}_{c}=\frac{n_{c}+\alpha-1}{n+k(\alpha-1)}$
- $\alpha=2$ gives Laplace smoothing (add 1 "fake" count for each class)


## Conjugate priors

- This is our second example where prior and posterior have the same form
- Beta prior + Bernoulli likelihood gives a Beta posterior
- Also happens with binomial, geometric, ... likelihoods
- Dirichlet prior + categorical likelihood gives a Dirichlet posterior
- Also happens with multinomial likelihood
- When this happens, we say prior is conjugate to the likelihood
- Prior and posterior come from the same "family" of distributions

$$
X \sim L(\theta) \quad \theta \sim P(\lambda) \quad \text { implies } \quad \theta \mid X \sim P\left(\lambda^{\prime}\right)
$$

- Updated parameters $\lambda$ will depend on the data
- Many computations become easier if we have a conjugate prior
- But not all distributions have conjugate priors
- And even when one exists, might not be convenient


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## Multi-class classification

- Often have classification with categorical labels and/or features

$$
\mathbf{X}=\left[\begin{array}{ccc}
\text { Cough } & \text { Low fever } & \text { Normal breathing } \\
\text { Cough } & \text { High fever } & \text { Shortness of breath } \\
\text { No cough } & \text { High fever } & \text { Normal breathing } \\
\text { No cough } & \text { Low fever } & \text { Normal breathing } \\
\text { Cough } & \text { Medium fever } & \text { Normal breathing }
\end{array}\right] \quad \mathbf{y}=\left[\begin{array}{c}
\text { Cold } \\
\text { Pneumonia } \\
\text { Covid } \\
\text { Covid } \\
\text { Cold }
\end{array}\right]
$$

- Can adapt all of our previous binary classification methods:
- Naïve Bayes
- Tabular probabilities
- Logistic regression / neural nets


## Product of categoricals, multi-class Naïve Bayes

- Start: multivariate categorical density estimation
- Input: $n$ iid samples of categorical vectors $x^{(1)}, \ldots, x^{(n)}$
- Output: model giving probability for any assignment of values $x_{1}, \ldots, x_{d}$

$$
\mathbf{X}=\left[\begin{array}{ccccccccc}
\mathrm{A} & \mathrm{C} & \mathrm{C} & \mathrm{~T} & \mathrm{~T} & \mathrm{~T} & \mathrm{~A} & \mathrm{G} & \mathrm{C} \\
\mathrm{~A} & \mathrm{C} & \mathrm{C} & \mathrm{G} & \mathrm{~T} & \mathrm{~T} & \mathrm{~A} & \mathrm{G} & \mathrm{G} \\
\mathrm{~A} & \mathrm{C} & \mathrm{C} & \mathrm{~T} & \mathrm{~T} & \mathrm{~T} & \mathrm{~A} & \mathrm{G} & \mathrm{C} \\
\mathrm{~A} & \mathrm{~A} & \mathrm{C} & \mathrm{~T} & \mathrm{~T} & \mathrm{~T} & \mathrm{C} & \mathrm{G} & \mathrm{G}
\end{array}\right] \xrightarrow{\text { density estimator }} \operatorname{Pr}\left(X_{1}=\mathrm{A}, X_{2}=\mathrm{C}, \ldots, X_{9}=\mathrm{C}\right)=0.11
$$

- Like for product of Bernoullis, we could use product of categoricals
- Assumes $X_{j}$ are mutually independent: strong assumption that makes things easy

$$
\operatorname{Pr}\left(X_{1}=c_{1}, \ldots, X_{d}=c_{d}\right)=\operatorname{Pr}\left(X_{1}=c_{1}\right) \ldots \operatorname{Pr}\left(X_{d}=c_{d}\right)=\theta_{1, c} \cdots \theta_{d, c_{d}}
$$

- Parameter $\theta_{j, c}$ is probability that $j$ th entry is in $c$ th class
- Like before, could use product of categoricals conditional on $Y$ to get categorical naïve Bayes


## Multi-class naïve Bayes on MNIST

- Binarized MNIST: label is categorical, but images are still product of Bernoullis
- Parameter of the Bernoulli for each class:

- One sample from each class:
为


## Tabular probabilities for categorical data

- Can use a tabular parameterization: with two binary features, three-way label,

$$
\begin{array}{llll}
\operatorname{Pr}\left(Y=1 \mid X_{1}=0, X_{2}=0\right)=\theta_{1 \mid 00} & \operatorname{Pr}\left(Y=2 \mid X_{1}=0, X_{2}=0\right)=\theta_{2 \mid 00} & \operatorname{Pr}\left(Y=3 \mid X_{1}=0, X_{2}=0\right)=\theta_{3 \mid 00} \\
\operatorname{Pr}\left(Y=1 \mid X_{1}=0, X_{2}=1\right)=\theta_{1 \mid 01} & \operatorname{Pr}\left(Y=2 \mid X_{1}=0, X_{2}=1\right)=\theta_{2 \mid 01} & \operatorname{Pr}\left(Y=3 \mid X_{1}=0, X_{2}=1\right)=\theta_{3 \mid 01} \\
\operatorname{Pr}\left(Y=1 \mid X_{1}=1, X_{2}=0\right)=\theta_{1 \mid 10} & \operatorname{Pr}\left(Y=2 \mid X_{1}=1, X_{2}=0\right)=\theta_{2 \mid 10} & \operatorname{Pr}\left(Y=3 \mid X_{1}=1, X_{2}=0\right)=\theta_{3 \mid 10} \\
\operatorname{Pr}\left(Y=1 \mid X_{1}=1, X_{2}=1\right)=\theta_{1 \mid 11} & \operatorname{Pr}\left(Y=2 \mid X_{1}=1, X_{2}=1\right)=\theta_{2 \mid 11} & \operatorname{Pr}\left(Y=3 \mid X_{1}=1, X_{2}=1\right)=\theta_{3 \mid 11}
\end{array}
$$

- Don't necessarily need $\theta_{3 \mid x}$; can use $\theta_{3 \mid x}=1-\theta_{1 \mid x}-\theta_{2 \mid x}$
- MLE has simple closed form: $\hat{\theta}_{y \mid x}=n_{y \mid x} / n_{x}$
- Just the categorical MLE for each condition
- Can use a Dirichlet (or whatever other) prior and do MAP
- Will overfit unless you have small number of distinct $x$


## Parameterizing conditionals

- Tabular treats each $\theta_{y \mid x}$ totally separately
- Could instead share information for "similar" $x$
- Can no longer express every possible distribution, potentially computationally harder
- Statistically much easier to fit
- One choice: weight $w_{c}$ for each class, get $z_{c}=w_{c}^{\top} x$ for each $c$
- Need to turn the $z_{c}$ into parameters of a categorical distribution
- Binary data: mapped one $z$ into $(0,1)$ with sigmoid $f(z)=1 /(1+\exp (-z))$
- But using $\theta_{c}=f\left(z_{c}\right)$ won't sum to one
- Softmax function first makes nonnegative by taking exp, then normalizes:

$$
\theta_{c}=[\operatorname{softmax}(\mathbf{z})]_{c}=\frac{\exp \left(z_{c}\right)}{\sum_{c^{\prime}=1}^{k} \exp \left(z_{c^{\prime}}\right)} \propto \exp \left(z_{c}\right)
$$

- Don't have to use softmax, other options exist, but this is default


## Categorical features as inputs

- How do we use categorical data in the features $x$ ?
- Usually convert to set of binary features ("one-hot" / "one of $k$ " encoding)

| Age | City | Income |  | Age | Van | Bur | Sur | Income |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 23 | Van | 26,000 |  | 23 | 1 | 0 | 0 | 26,000 |
| 25 | Sur | 67,000 | $\rightarrow$ | 25 | 0 | 0 | 1 | 67,000 |
| 19 | Bur | 16,500 |  | 19 | 0 | 1 | 0 | 16,500 |
| 43 | Sur | 183,000 |  | 43 | 0 | 0 | 1 | 183,000 |

- If you see a new category in test data: usually, just set all of them to zero


## Softmax and binary logistic regression

- With two categories: using a "dummy" value $z_{2}=0$

$$
[\operatorname{softmax}((z, 0))]_{1}=\frac{\exp (z)}{\exp (z)+\exp (0)} \times \frac{\exp (-z)}{\exp (-z)}=\frac{1}{1+\exp (-z)}
$$

- Two-class softmax regression with one weight frozen at zero is logistic regression


## Softmax loss

- Taking the negative log-likelihood:

$$
\begin{aligned}
-\log p(\mathbf{y} \mid W, \mathbf{X}) & =-\sum_{i=1}^{n} \log p\left(y^{(i)} \mid W, x^{(i)}\right)=-\sum_{i=1}^{n}\left[\log \left(\frac{\exp \left(w_{y^{(i)}}^{\top} x^{(i)}\right)}{\sum_{c=1}^{k} \exp \left(w_{c}^{\top} x^{(i)}\right)}\right)\right] \\
& =\sum_{i=1}^{n}\left[-w_{y^{(i)}}^{\top} x^{(i)}+\log \left(\sum_{c=1}^{k} \exp \left(w_{c}^{\top} x^{(i)}\right)\right]\right.
\end{aligned}
$$

- Convex (note log-sum-exp is convex), differentiable: can use gradient descent - Often add a regularizer (i.e. a prior on $W$ )
- Gradient has a nice form:

$$
\frac{\partial}{\partial w_{c}}[-\log p(\mathbf{y} \mid W, \mathbf{X})]=-\sum_{i=1}^{n} \mathbb{1}\left(y^{(i)}=c\right) x^{(i)}+\sum_{i=1}^{n} \underbrace{\frac{\exp \left(w_{c}^{\top} x^{(i)}\right)}{\sum_{c^{\prime}=1}^{k} \exp \left(w_{c^{\prime}}^{\top} x^{(i)}\right)}}_{p\left(y^{(i)}=c \mid x^{(i)}, W\right)} x^{(i)}
$$

## Multi-label versus multi-class classification

- Before: we saw multi-label classification, where $y$ is a binary vector of length $k$
- "This image has a chair and a person, but no frog"
- Multi-class, e.g. with softmax loss: $y$ has exactly one of $k$ discrete labels
- "This is an image of a frog"
- Could have multiple categorical labels (some of which might be binary)
- "This paper's arXiv primary class is stat.ML, and the first author is a student"


## Summary

- Monte Carlo is a general way to estimate expectations when you can sample - Including probabilities: expectations of indicators
- Next time: everything is regularization


## Law of the Unconscious Statistician

- These inequalities sometimes called "Law of the Unconscious Statistician":

$$
\mathbb{E}[g(X)]=\sum_{x \in \mathcal{X}} g(x) p(x) \quad \mathbb{E}[g(X)]=\int_{x \in \mathcal{X}} g(x) p(x) \mathrm{d} x
$$

- Two explanations I've heard for "unconscious":
- You can compute expectations without thinking
- Or: people don't realize this is actually a theorem to prove, not a definition

$$
Y=g(X)
$$

$$
\mathbb{E}[Y]=\sum_{y} y \operatorname{Pr}(Y=y)=\sum_{y} y \sum_{x: g(x)=y} p(x)=\sum_{x} g(x) p(x)
$$

## Mean and Variance of Monte Carlo

- $\hat{\mu}=\frac{1}{n} \sum_{i=1}^{n} g\left(x^{(i)}\right)$ is an unbiased estimate of $\mu=\mathbb{E}[g(x)]$ :

$$
\mathbb{E}\left[\frac{1}{n} \sum_{i=1}^{n} g\left(x^{(i)}\right)\right]=\frac{1}{n} \sum_{i=1}^{n} \mathbb{E}\left[g\left(x^{(i)}\right)\right]=\frac{1}{n} \sum_{i=1}^{n} \mu=\mu
$$

- If $\operatorname{Var}\left(g\left(x^{(i)}\right)\right)=\sigma^{2}$ for some finite $\sigma$, then

$$
\begin{aligned}
\operatorname{Var}\left(\frac{1}{n} \sum_{i=1}^{n} g\left(x^{(i)}\right)\right) & =\frac{1}{n^{2}} \sum_{i=1}^{n} \underbrace{\operatorname{Var}\left(g\left(x^{(i)}\right)\right)}_{\sigma^{2}}-\frac{2}{n^{2}} \sum_{i \neq j} \underbrace{\operatorname{Cov}\left(g\left(x^{(i)}\right), g\left(x^{(j)}\right)\right)}_{0} \\
& =\frac{1}{n^{2}} n \sigma^{2}=\frac{\sigma^{2}}{n}
\end{aligned}
$$

- Expected squared error is $\sigma^{2} / n$ :

$$
\mathbb{E}\left[\left(\frac{1}{n} \sum_{i=1}^{n} g\left(x^{(i)}\right)-\mu\right)^{2}\right]=\left(\mathbb{E} \frac{1}{n} \sum_{i=1}^{n} g\left(x^{(i)}\right)-\mu\right)^{2}+\operatorname{Var}\left(\frac{1}{n} \sum_{i=1}^{n} g\left(x^{(i)}\right)\right)=0+\frac{\sigma^{2}}{n}
$$

Monte Carlo as a stochastic gradient method

Can view as SGD on $f(\hat{\mu})=\frac{1}{n}\|\hat{\mu}-\mu\|^{2}$ with learning rate $\frac{1}{i+1}$ :

$$
\begin{aligned}
\hat{\mu}_{n} & =\hat{\mu}_{n-1}-\frac{1}{n}\left(\hat{\mu}_{n-1}-x^{(i)}\right) \\
& =\left(1-\frac{1}{n}\right) \hat{\mu}_{n-1}+\frac{1}{n} x^{(i)} \\
& =\frac{n-1}{n}\left(\frac{1}{n-1} \sum_{i=1}^{n-1} x^{(i)}\right)+\frac{1}{n} x^{(i)} \\
& =\frac{1}{n} \sum_{i=1}^{n-1} x^{(i)}+\frac{1}{n} x^{(i)}=\frac{1}{n} \sum_{i=1}^{n} x^{(i)}
\end{aligned}
$$

