Quiz Review

CMPUT 367: Intermediate Machine Learning

Comments

- The goal of the exam is to test (a) did you understand the basic ideas and (b) can you apply that understanding
- Answers can be relatively short, say at most 5 sentences
- I will mark these and will look for your thought process. As this is the second time this course is taught, I will err on the side of being generous; so help me out by letting me see how you reasoned about the question

Ch 2: Probability Basics

- Expectations and variance
- Independence and conditional independence
- Joint probabilities, marginal and conditional probabilities
- **You will not yet be tested on**
  - Mixtures of distributions
  - KL divergences to compare distributions

Some questions (1)

- Assume $\mathbf{X}$ is a random vector of dimension d, with covariance $\mathbf{\Sigma}$
- **Question**: Does this mean $\mathbf{X}$ is a multivariate Gaussian? Why or why not?

Some questions (2)

- Assume $\mathbf{X}$ is a random vector of dimension d, with covariance $\mathbf{\Sigma}$
- **Question**: Does this mean $\mathbf{X}$ is a multivariate Gaussian? Why or why not?
- **Answer**: No, covariance is defined for any of the distributions we talk about. The variable $\mathbf{X}$ can even consist of both continuous and discrete random variables

Some questions (3)

- Assume $\mathbf{X}$ is a random vector of dimension d, with covariance $\boldsymbol{\Sigma}$
- **Follow-up question**: If X_1 is continuous and X_2 is discrete, then what is the formula for Cov(X_1, X_2) ?
- Recall: Cov$(X_1, X_2) = \mathbb{E}[(X_1 - \mathbb{E}[X_1])(X_2 - \mathbb{E}[X_2])]$

Some questions (4)

- Assume $\mathbf{X}$ is a random vector of dimension d, with covariance $\mathbf{\Sigma}$
- **Follow-up**: If X_1 is continuous and X_2 is discrete, then what is the formula for Cov(X_1, X_2) ?
- **Answer**: Let μ_1 and μ_2 be the means for X_1 and X_2 respectively

$$\text{Cov}(X_1, X_2) = \mathbb{E}[(X_1 - \mathbb{E}[X_1])(X_2 - \mathbb{E}[X_2])]$$

$$= \int_{\mathcal{X}_1} \sum_{x_2 \in \mathcal{X}_2} p(x_1, x_2)(x_1 - \mu_1)(x_2 - \mu_2) dx_1$$

- $$= \int_{\mathcal{X}_1} p(x_1) \sum_{x_2 \in \mathcal{X}_2} p(x_2 \mid x_1)(x_1 - \mu_1)(x_2 - \mu_2) dx_1$$

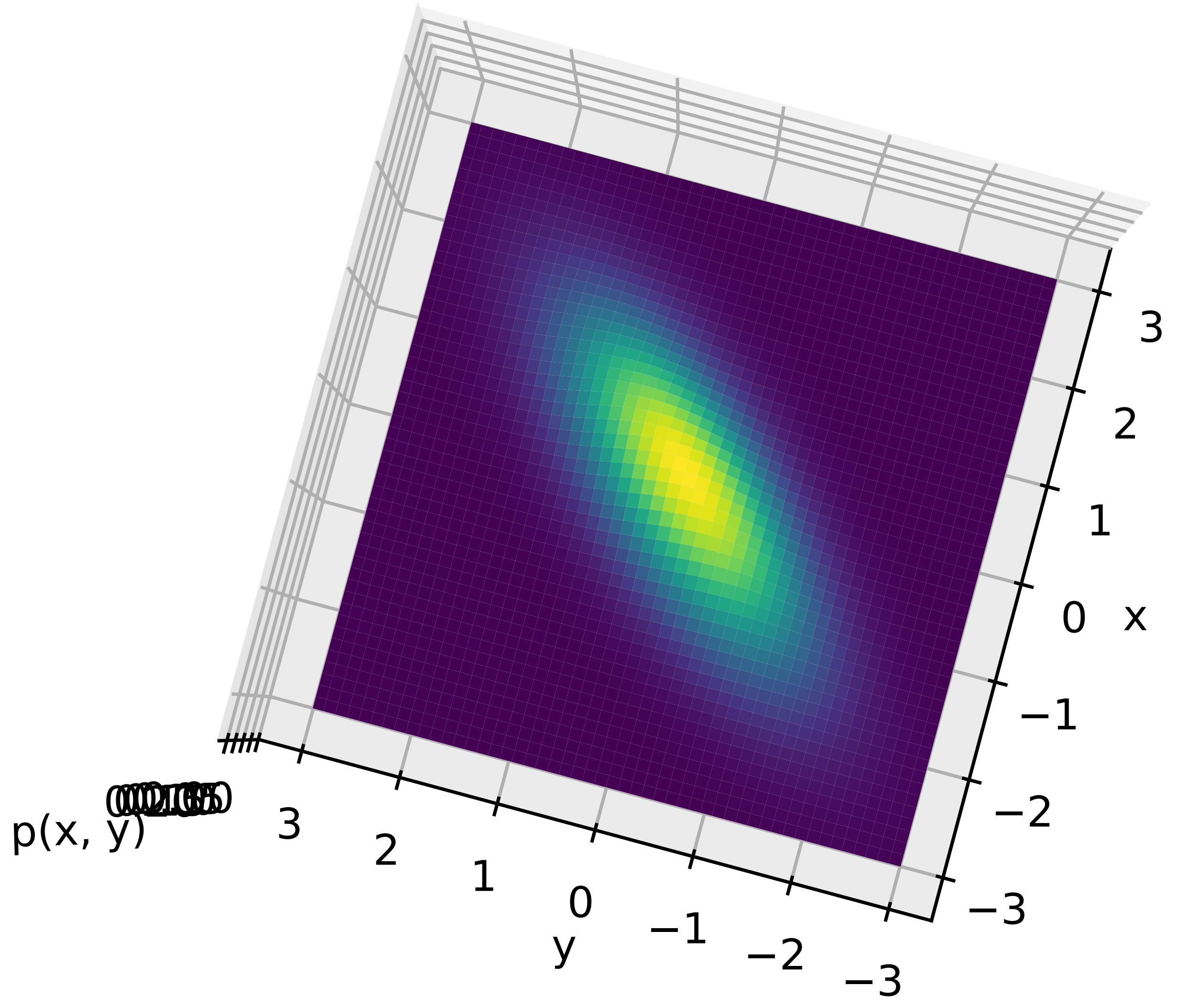
Some questions (5)

- Assume $\mathbf{X}$ is a random vector of dimension d, with covariance $\mathbf{\Sigma}$
- Now assume $\mathbf{X}$ is a multivariate Gaussian
- **Question**: If the first eigenvalue in $\mathbf{\Sigma}$ is very big (1000) and the second is very small (0.1), then what does this tell us about the shape of the Gaussian?

Some questions (5)

- Assume $\mathbf{X}$ is a random vector of dimension d, with covariance $\mathbf{\Sigma}$
- Now assume $\mathbf{X}$ is a multivariate Gaussian
- **Question**: If the first eigenvalue in $\mathbf{\Sigma}$ is very big (1000) and the second is very small (0.1), then what does this tell us about the shape of the Gaussian?
- **Answer**: The distribution is wide in one orientation and narrow in another

Example of eigenvalues



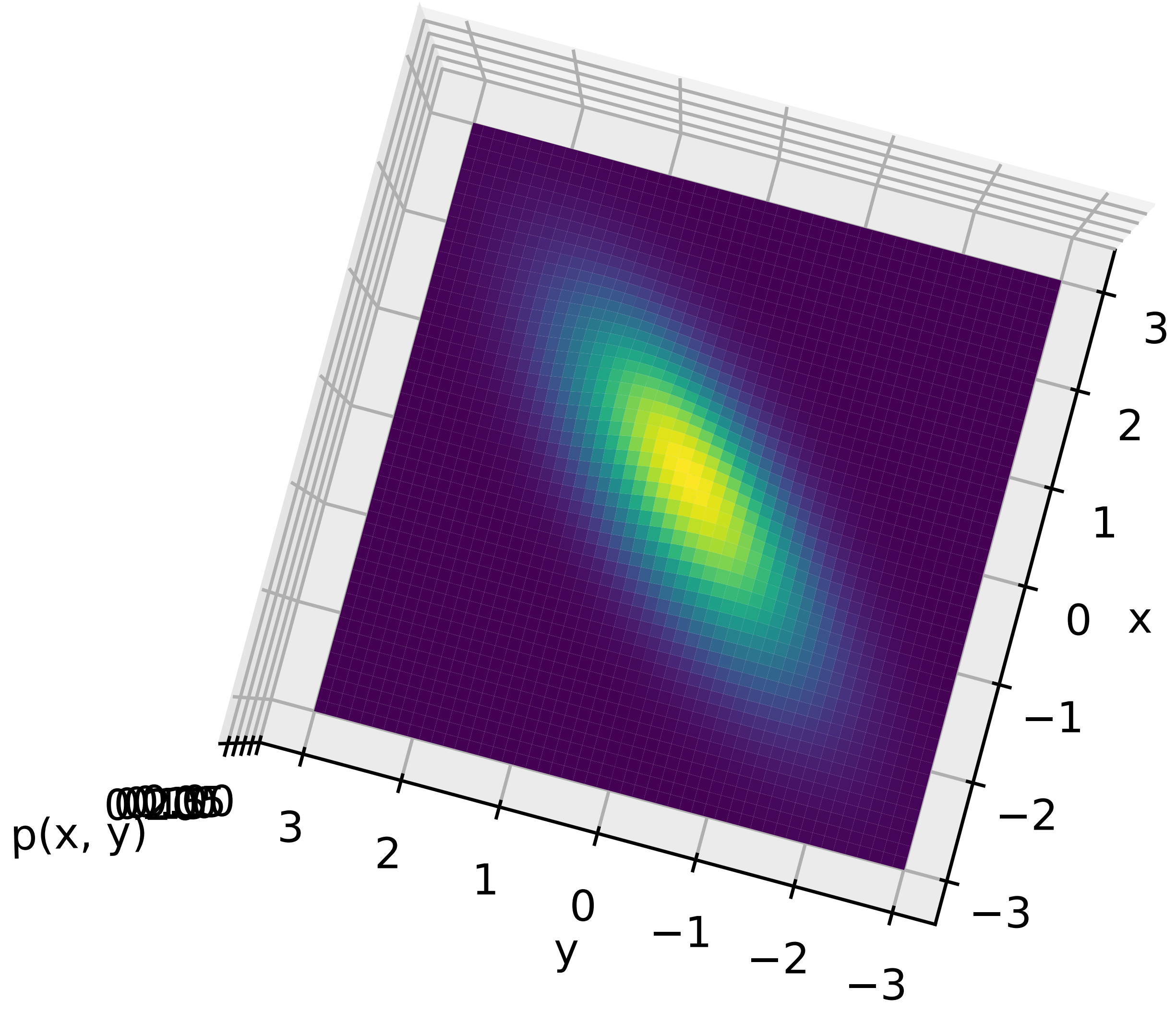
$$\boldsymbol{\Sigma} = \begin{bmatrix} 1.0 & 0.75 \\ 0.75 & 1.0 \end{bmatrix}$$

This $\boldsymbol{\Sigma}$ has singular values: $\sigma_1 = 1.75, \sigma_2 = 0.25$

These are also the eigenvalues for $\boldsymbol{\Sigma}$!

This is not true in general. Why is is true for $\boldsymbol{\Sigma}$?

Example of eigenvalues



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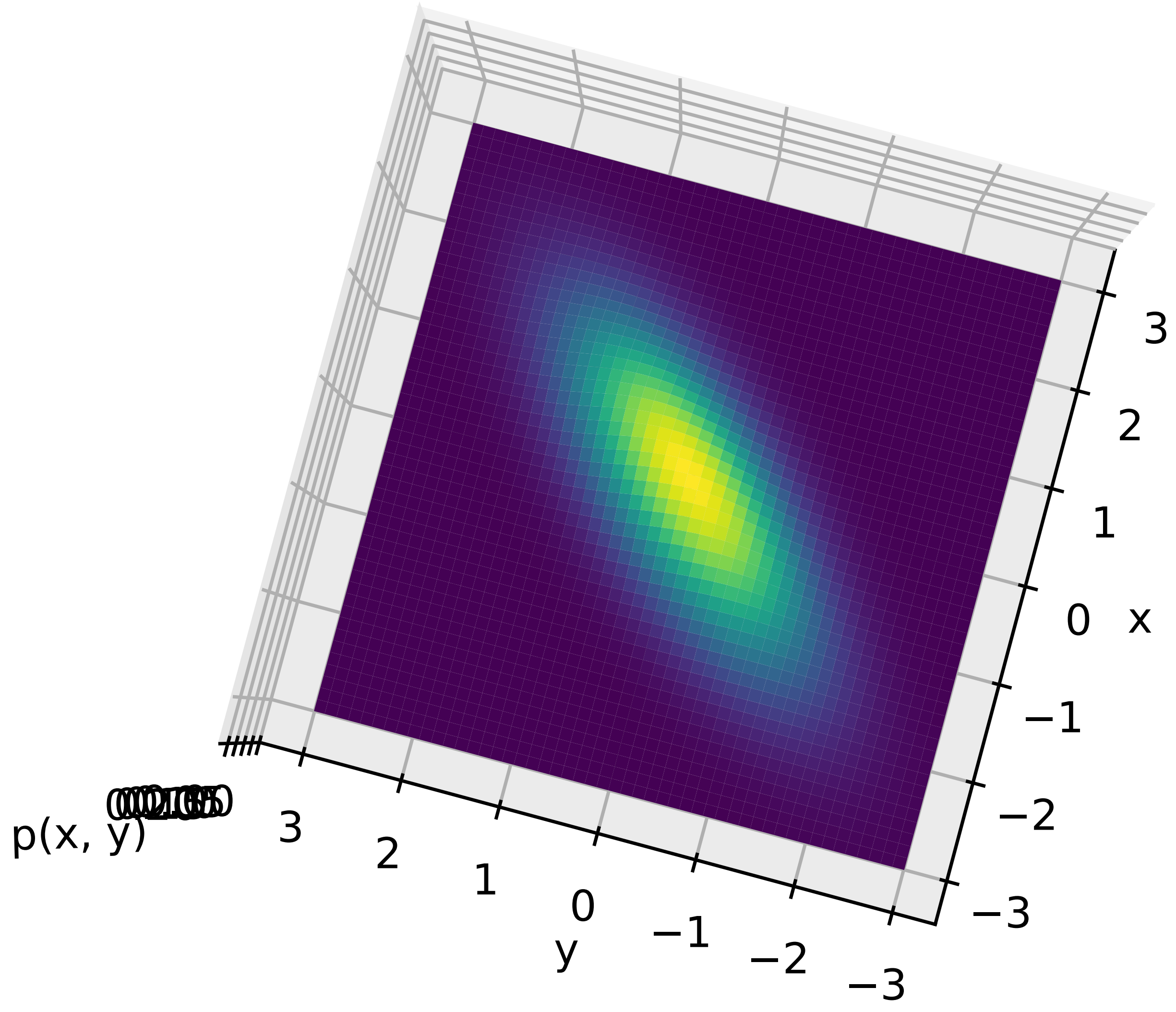
For a square, symmetric matrix, the eigenvalue decomposition is

$\mathbf{\Sigma} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\top$ for orthonormal $\mathbf{U}$, diagonal $\mathbf{\Lambda}$

We also know $\mathbf{\Sigma}$ is positive definite. What does this tell us about $\mathbf{\Lambda}$?

Example of eigenvalues



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For a square, symmetric matrix, the eigenvalue decomposition is

$\mathbf{\Sigma} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\top$ for orthonormal $\mathbf{U}$, diagonal $\mathbf{\Lambda}$

$\mathbf{\Sigma}$ is positive definite, so $\mathbf{\Lambda}$ is a diagonal matrix with positive terms on the diagonal

Therefore, $\mathbf{\Sigma} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\top$ is also a valid SVD

Ch 3: Revisiting Linear Regression

- Linear regression objective and closed-form matrix solution (OLS)
  - but you don't need to remember the formula
- Understanding why small singular values can indicate we get overfitting
- The utility of l2 regularization for avoiding issues with small singular values
- The bias-variance trade-off, and relationship to the covariance matrix and the singular values of the data matrix

Linear Regression Objectives

- LR objective $\frac{1}{2}||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2 = \frac{1}{2}\sum_{i=1}^{n}(\mathbf{x}_i^\top \mathbf{w} - y_i)^2$
- Ridge Regression objective $\frac{1}{2}||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2 + \frac{\lambda}{2}||\mathbf{w}||_2^2$
- **Question**: How do we get the LR objective from the RR objective?

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- Ridge Regression objective $\frac{1}{2}\|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2 + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$
- **Question**: How do we get the LR objective from the RR objective?
- **Answer**: Set $\lambda = 0$ (regularization weight is zero, so no regularizer)

Linear Regression Solution

- The closed form solution satisfies $\mathbf{A}\mathbf{w} = \mathbf{b}$ for $\mathbf{A} = \mathbf{X}^\top \mathbf{X}$ and $\mathbf{b} = \mathbf{X}^\top \mathbf{y}$
- **Question**: Our goal is to minimize $\frac{1}{2}||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2$. Why can't we just use $\mathbf{w} = \mathbf{X}^{-1}\mathbf{y}$? This would be great because then we would have $\mathbf{X}\mathbf{w} = \mathbf{y}$

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- **Question**: Our goal is to minimize $\frac{1}{2}||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2$. Why can't we just use $\mathbf{w} = \mathbf{X}^{-1}\mathbf{y}$? Then we would have $\mathbf{X}\mathbf{w} = \mathbf{y}$
- **Answer**: $\mathbf{X}$ is typically not a square matrix and so cannot be inverted (inverse only exists for square matrices)
- Instead, the pseudo-inverse $\mathbf{X}^\dagger \in \mathbb{R}^{d\times n}$ is the closest we get to an inverse and $\mathbf{w} = \mathbf{X}^\dagger\mathbf{y}$ (here $\mathbf{X}^\dagger\mathbf{X} = \mathbf{I} \in \mathbb{R}^{d\times d}$ if $\mathbf{X}$ full rank, but $\mathbf{X}\mathbf{X}^\dagger \neq \mathbf{I} \in \mathbb{R}^{n\times n}$)
- Notice $\mathbf{X}\mathbf{w} = \mathbf{X}\mathbf{X}^\dagger\mathbf{y} \neq \mathbf{y}$, but in some sense closest approximation

Linear Regression Solution and Overfitting

- The closed form solution satisfies $\mathbf{A}\mathbf{w} = \mathbf{b}$ for $\mathbf{A} = \mathbf{X}^\top\mathbf{X}$ and $\mathbf{b} = \mathbf{X}^\top\mathbf{y}$
- If $\mathbf{A}$ is low-rank ($\mathbf{X}$ has a zero singular values), then there are infinitely many solutions for $\mathbf{w}$
    - Namely this linear system is under-constrained
- More likely, $\mathbf{A}$ is nearly low-rank; equivalently $\mathbf{X}$ is nearly low-rank
- Typical reason: insufficient data
- In d dimensions, the observed data **looks** like it lies in a lower-dimensional space, because it takes many points to start covering the actual region spanned by the data

LR and Overfitting

- We know that $\mathbf{X}$ can have small singular values if
  - input features are highly correlated (or linearly dependent)
  - OR we have insufficient data
- **Question**: If the true y is only a function of the first two features of $\mathbf{x}$, then does that imply that $\mathbf{X}$ will be low rank?

LR and Overfitting

- We know that $\mathbf{X}$ can have small singular values if
  - input features are highly correlated (or linearly dependent)
  - OR we have insufficient data
- **Question**: If the true y is only a function of the first three features of $\mathbf{x}$, then does that imply that $\mathbf{X}$ will be low rank?
- **Answer**: likely not. They are different random variables. The functional relationship is about how the RVs $\mathbf{x}$ and y are related. It does not necessarily imply anything about the relationships between RVs within $\mathbf{x}$

LR and Overfitting

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- **Answer**: likely not. They are different random variables. The functional relationship is about how the RVs $\mathbf{x}$ and y are related. It does not necessarily imply anything about the relationships between RVs within $\mathbf{x}$
- **Exception**: y might only be a function of the first three features because the rest are all perfectly redundant. Then both y is only related to the first three features AND $\mathbf{X}$ is low rank. But there is no reason to believe this is the reason for the relationship, without further info

The LR solution, with and without regularization

- $\mathbf{w}_{\text{MLE}} = \sum_{j=1}^{\text{rank}(X)} \frac{\mathbf{u}_j^\top \mathbf{y}}{\sigma_j} \mathbf{v_j}$ for $\mathbf{w}_{\text{MLE}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$
- $\mathbf{w}_{\text{MAP}} = \sum_{j=1}^{\text{rank}(X)} \frac{\sigma_j \mathbf{u}_j^\top \mathbf{y}}{\sigma_j^2 + \lambda} \mathbf{v_j}$ for $\mathbf{w}_{\text{MAP}} = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}$
- If λ reasonably big (say 10^-3), then we avoid dividing by a very small singular value
- **Question**: Why do we subscript these with MLE and MAP?

Bias and variance

- $\mathbf{w}_{\text{MLE}}$ is unbiased and potentially high-variance, $\sigma^2\mathbb{E}\left[\sum_{j=1}^{d}\sigma_j^{-2}\right]$

- $\mathbf{w}_{\text{MAP}}$ is biased and lower variance, $\sigma^2\mathbb{E}\left[\sum_{j=1}^{d}\frac{\sigma_j^2}{(\sigma_j^2+\lambda)^2}\right]$

- **Question**: when do we expect $\mathbf{w}_{\text{MAP}}$ to be better than $\mathbf{w}_{\text{MLE}}$?

Bias and variance

- $\mathbf{w}_{\text{MLE}}$ is unbiased and potentially high-variance, $\sigma^2\mathbb{E}\left[\sum_{j=1}^{d}\sigma_j^{-1}\right]$
- $\mathbf{w}_{\text{MAP}}$ is biased and lower variance, $\sigma^2\mathbb{E}\left[\sum_{j=1}^{d}\frac{\sigma_j^2}{(\sigma_j^2+\lambda)^2}\right]$
- **Exercise**: show that the variance for $\mathbf{w}_{\text{MAP}}$ always lower than $\mathbf{w}_{\text{MLE}}$

Ch 3: Revisiting Linear Regression

- **You will not be tested on**
  - Predicting multiple outputs simultaneously
  - Using weighted error functions
  - The closed-form solutions for OLS or ridge regression (l2-regularized linear regression)
  - The formulas for bias and variance for OLS and ridge regression

Ch. 4: Optimization

- Second-order multivariate gradient descent
- Understanding why the Hessian in the second-order update accounts for differences in curvature in different dimensions
- Understanding the importance of an adaptive vector stepsize
- The mini-batch stochastic gradient descent (SGD) update rule
- Understanding why SGD is a more computationally efficient update than GD
- Understanding the momentum update

Ch. 4: Optimization

- **You will not be tested on**
- Remembering the formulas for momentum, RMSProp and Adam.
- **But you should at this point know** the second-order and first-order gradient descent and mini-batch SGD updates (these are very generic)
- You will not need to compute any Hessians

All the Updates

- Assumes we have $c(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n} c_i(\mathbf{w})$

- Second-order GD: $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \mathbf{H}^{-1}_{c(w_t)} \nabla c(\mathbf{w}_t)$

- First-order GD with vector stepsizes: $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \boldsymbol{\eta}_t \cdot \nabla c(\mathbf{w}_t)$
  - element-wise product with stepsize

- Mini-batch SGD with vector stepsizes, using a mini-batch $\mathscr{B}$ of indices: $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \boldsymbol{\eta}_t \cdot \frac{1}{b}\sum_{i \in \mathscr{B}} \nabla c_i(\mathbf{w}_t)$

Some optimization questions

- We use $c(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n} c_i(\mathbf{w})$. But when we did LR we used $c(\mathbf{w}) = \sum_{i=1}^{n} c_i(\mathbf{w}) = \frac{1}{2}\|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2$. Is this mismatch a problem?
- How do we write the Ridge Regression loss as $c(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n} c_i(\mathbf{w})$?

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- **Answer**: the constant 1/n in front does not change the solution. For OLS, it is really not necessary to include 1/n. When talking about GD and SGD, its useful to think of c as an expectation over losses per sample
- Though even for OLS it can be useful to normalize

Extra: What is the OLS solution for the normalized objective?

- $c(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n} c_i(\mathbf{w}) = \frac{1}{2n}\|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2$ gives gradients
- $\frac{1}{n}\mathbf{X}^\top\mathbf{X}\mathbf{w} = \frac{1}{n}\mathbf{X}^\top\mathbf{y}$ and so $\mathbf{w} = \left(\frac{1}{n}\mathbf{X}^\top\mathbf{X}\right)^{-1}\frac{1}{n}\mathbf{X}^\top\mathbf{y}$
- Notice that the 1/n comes outside the inverse and becomes n
- $\mathbf{w} = \left(\frac{1}{n}\mathbf{X}^\top\mathbf{X}\right)^{-1}\frac{1}{n}\mathbf{X}^\top\mathbf{y} = n\left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\frac{1}{n}\mathbf{X}^\top\mathbf{y} = \left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\mathbf{X}^\top\mathbf{y}$

Some optimization questions

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- How do we write the Ridge Regression loss as $c(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n} c_i(\mathbf{w})$?

A normalized RR objective

- $\frac{1}{2}\|\mathbf{X}\mathbf{w}-\mathbf{y}\|_2^2+\frac{\lambda}{2}\|\mathbf{w}\|_2^2$. What is the normalized c?
- $c(\mathbf{w})=\frac{1}{n}\sum_{i=1}^{n}c_i(\mathbf{w})=\frac{1}{2n}\|\mathbf{X}\mathbf{w}-\mathbf{y}\|_2^2+\frac{\lambda}{2n}\|\mathbf{w}\|_2^2=\frac{1}{n}\left(\frac{1}{2}\|\mathbf{X}\mathbf{w}-\mathbf{y}\|_2^2+\frac{\lambda}{2}\|\mathbf{w}\|_2^2\right)$
- Therefore must have $c_i(\mathbf{w})=\frac{1}{2}(\mathbf{x}_i^\top\mathbf{w}-y_i)^2+\frac{\lambda}{2}\|\mathbf{w}\|_2^2$
- Makes very clear that regularizer has a diminishing role with increasing n

A normalized RR objective

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- Makes very clear that regularizer has a diminishing role with increasing n
- **Question**: What is the mini-batch SGD update for RR?

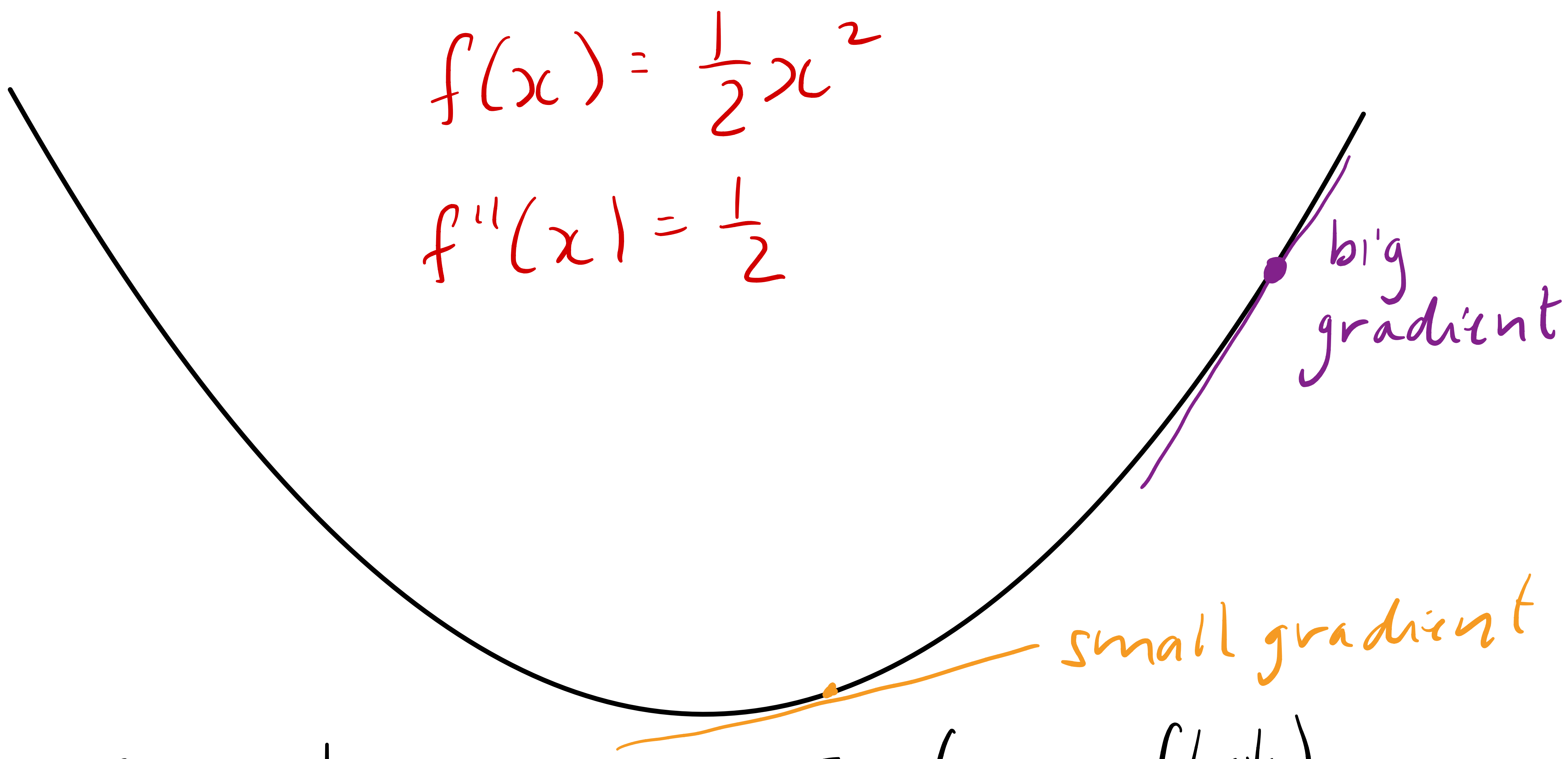
Mini-batch SGD for RR

- Therefore must have $c_i(\mathbf{w}) = \frac{1}{2}(\mathbf{x}_i^\top \mathbf{w} - y_i)^2 + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$
- **Question**: What is the mini-batch SGD update for RR?
- $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \boldsymbol{\eta}_t \cdot \frac{1}{b} \sum_{i \in \mathscr{B}} \nabla c_i(\mathbf{w}_t)$
- where $\nabla c_i(\mathbf{w}) = (\mathbf{x}_i^\top \mathbf{w} - y_i)\mathbf{x}_i + \lambda \mathbf{w}$

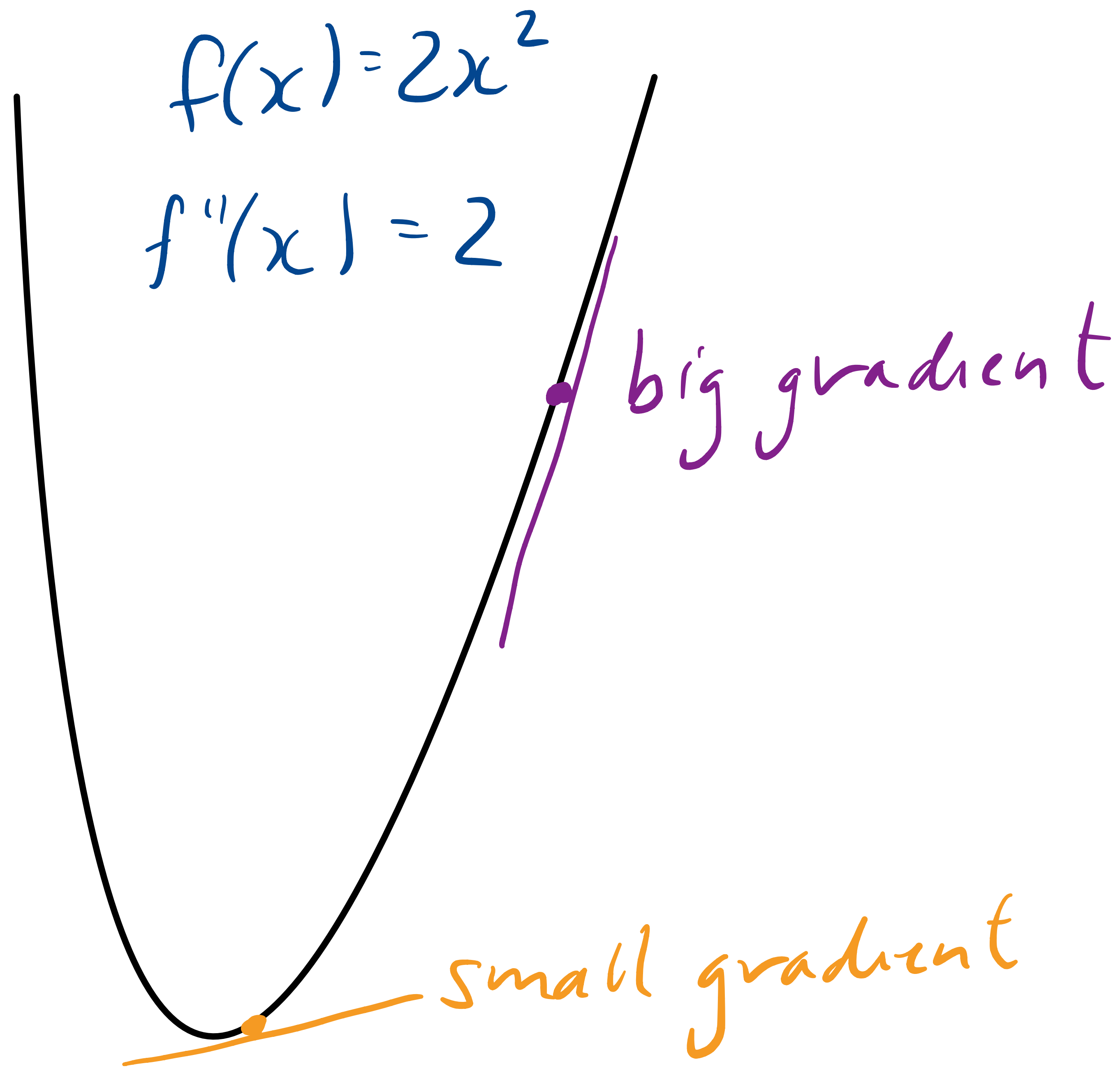
The Hessian and curvature

- The Hessian and second-derivative have a clear correspondence using the directional derivative
- The curvature (second-derivative) is about the shape of the bowl (wide flat bowl, or steep bowl)
- The gradient is at a specific point in that bowl, and can be big or small

Visualizing the difference



Curvature is 0.5 (more flat)



Curvature is 2.0 (more steep).

Second-order stepsize is always 2 here, for both gradients

Second-order stepsize is always 0.5 here, for both gradients

The Hessian has two uses

- The Hessian also helps us know: are we in a local-min, local-max or potentially a saddlepoint?
- But this question only uses the sign of the eigenvalues of the Hessian. The magnitudes give additional information (about curvature)
  - Signs tell us type of bowl (convex or concave)
  - Magnitudes tells us the shape of the bowl
- We care more about Hessian approximations to approximate curvature

Momentum

- Replaces update with an exponential average of gradients
- $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta_t \cdot \mathbf{g}_t$ becomes $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta_t \cdot \mathbf{m}_{t+1}$ for either
- $\mathbf{m}_{t+1} = \mathbf{g}_t + \beta \mathbf{m}_t$ or normalized $\mathbf{m}_{t+1} = (1-\beta)\mathbf{g}_t + \beta \mathbf{m}_t$
- Smooths descent direction

Normalizing the momentum

- Equivalent to use $\mathbf{m}_{t+1} = \mathbf{g}_t + \beta \mathbf{m}_t$ or normalized $\mathbf{m}_{t+1} = (1-\beta)\mathbf{g}_t + \beta \mathbf{m}_t$
- To get the normalized one, equivalent to use $\mathbf{m}_{t+1} = \mathbf{g}_t + \beta \mathbf{m}_t$ and then normalize $(1-\beta)\mathbf{m}_{t+1}$; the normalization absorbed into the stepsize η
- Notice $\mathbf{m}_{t+1} = \mathbf{g}_t + \beta \mathbf{m}_t = \mathbf{g}_t + \beta \mathbf{g}_{t-1} + \beta^2 \mathbf{m}_{t-1} = \ldots = \sum_{i=0}^{t} \beta^i \mathbf{g}_{t-i}$
- $\mathbf{m}_{t+1} = (1-\beta)\mathbf{g}_t + \beta \mathbf{m}_t = (1-\beta)\mathbf{g}_t + \beta(1-\beta)\mathbf{g}_{t-1} + \beta^2 \mathbf{m}_{t-1} = \ldots = (1-\beta)\sum_{i=0}^{t} \beta^i \mathbf{g}_{t-i}$

Momentum vs RMSProp

- RMSProp slows down descent if several big gradients in a row
- Momentum seems to accelerate if so. What’s the deal?

Momentum vs RMSProp

- RMSProp slows down descent if several big gradients in a row
- Momentum seems to accelerate if so. What’s the deal?
- **Answer**: we should think of momentum actually more as dampening.
- It takes an average of gradient, so it doesn’t really accumulate large values (as long as we normalize, or make the stepsize out in front a bit smaller)
- But it nicely avoids oscillating when gradients change signs
- RMSProp does not as effectively prevent oscillation, since it just uses magnitude not sign

Ch. 5: Generalized Linear Models

- Understand the purpose of the generalization from linear regression to GLMs
- Understand that the exponential family distribution underlies GLMs
- Know that linear regression, Poisson regression, logistic regression and multinomial logistic regression are examples of GLMs
- Know the distributions and transfers that correspond to each of these four GLMs
    - e.g., Poisson regression has a Poisson distribution $p(y \mid x)$ with transfer exp

Generalized Linear Models (GLMs)

- Generalizes linear regression and p(y | x) a Gaussian: allows p(y |x) to be any natural exponential family distribution with natural parameter $\theta(x)$
- In GLMs, we learn the natural parameter $\theta(x) = x^\top w$
- Then $\mathbb{E}[Y|x] = g(\theta(x))$ for transfer function g
  - e.g., Gaussian with fixed (unknown) variance has g = identity
  - e.g., Bernoulli has $g = \sigma$ (i.e., $\sigma(\theta(x)) = \mathbb{E}[Y|x]$)
  - e.g., Poisson p(y | x) has $g = \exp$
  - e.g., Multinomial (categorial) p(y | x) for multi-class has g = softmax

Exponential Family Distribution

- Generalize from $p(y \mid \mathbf{x}) = \mathcal{N}(\mathbf{x}^\top \mathbf{w}, \sigma^2)$ to a wider set of distributions
- $p(y \mid \mathbf{x}) = \exp(\theta(\mathbf{x})y - a(\theta(\mathbf{x})) + b(y))$ for $\theta(\mathbf{x}) = \mathbf{x}^\top \mathbf{w}$
- More generally, y can also be multivariate giving. Let $\mathbf{y}$ be a row vector.
- $p(\mathbf{y} \mid \mathbf{x}) = \exp(\langle \theta(\mathbf{x}), \mathbf{y} \rangle - a(\theta(\mathbf{x})) + b(y))$ for $\theta(\mathbf{x}) = \mathbf{x}\mathbf{W}$
- and where the log-partition function a inputs vectors instead of scalars
- For these distributions, using $g = \nabla a$ and $\theta(\mathbf{x}) = \mathbf{x}\mathbf{W}$ with log-likelihood results in a convex optimization

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- and where the log-partition function a inputs vectors instead of scalars
- For these distributions, using $g = \nabla a$ and $\theta(\mathbf{x}) = \mathbf{x}\mathbf{W}$ with log-likelihood results in a convex optimization
- Question: why is it useful that this is a convex optimization?

Switch to whiteboard and practice quiz

- The practice quiz cover the remaining review