Final Review

CMPUT 467/567: Machine Learning II

Winter 2026
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Goal of these Slides

- Go over each section of the notes and highlight key concepts
- Additionally highlight what I will and will not test
  - It is in the notes for your knowledge, but hard to directly test
- Practice Final will be covered in a later session, closer to the actual final
- Note: the final largely focuses on Chapter 10 onwards. But as usual it builds on your knowledge from earlier chapters

Chapter 1: Intro to ML

- Know the difference between a generative model and predictor (1.1)
- **Will not be directly tested:**
  - Relationship to Statistics and Probability (1.2)
  - The Blessing and Curse of Dimensionality (1.3)
  - SVDs and Eigenvalue decompositions (1.4)

Chapter 2: Probability Concepts

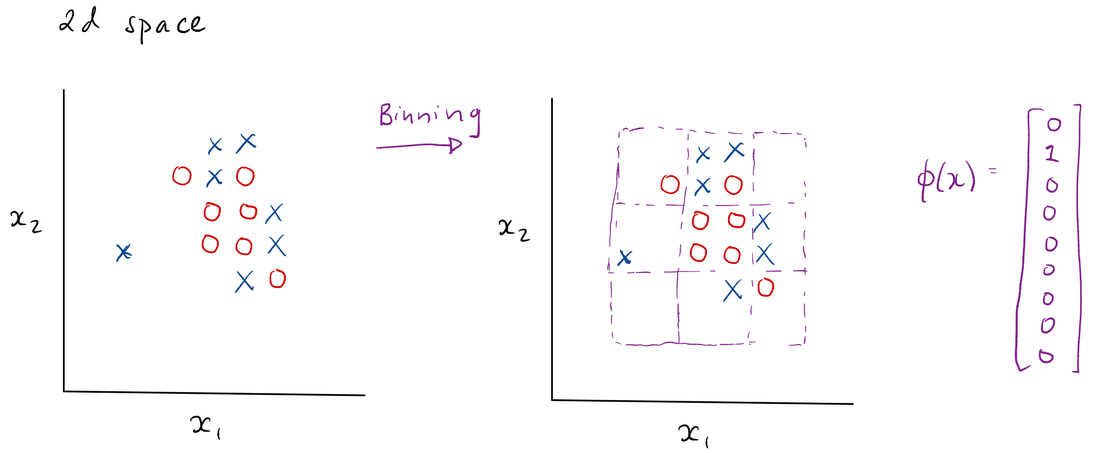
- Understand the definition of a multi-dimensional probability (2.1)
- Understand the definition of a mixture of distributions (2.2)
- Know the purpose of the KL divergence (2.3)
- **Will not be directly tested:**
  - Knowing the PMFs or PDFs of specific distributions
  - Specific expectation and variance formulas
  - Remembering the KL divergence formula

Chapter 3: Fixed Representations

- We discussed polynomials, RBF Networks and Prototype representations
- We discussed how these fixed representations allow us to learn nonlinear functions
- **Will not test**
  - Any representability results for these functions
  - Specific formulas for kernels

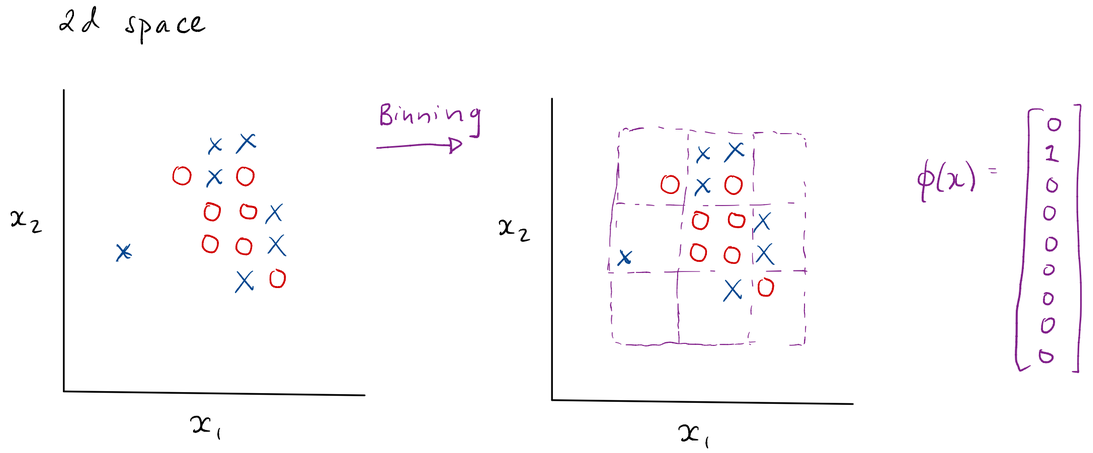
Exercise

- I didn’t give you an example of how projecting to higher dimensions also facilitates regression with simple (linear functions)
- Can you think of a similar example to this one, but for regression?



Exercise

- I didn't give you an example of how projecting to higher dimensions also facilitates regression with simple (linear functions)
- Can you think of a similar example to this one, but for regression?
  - Same ϕ lets us learn an average y per bin
  - Can also use a linear function per bin, by using (x1,x2) per bin, giving piecewise linear functions
    - e.g., bin 1: [x1, x2, 0, 0, 0, ….]
      bin 2: [0, 0, x1, x2, 0, 0, ….]



Ch 4: Revisiting Generalization Error

- The definition of generalization error (expected cost)
- Overfitting and underfitting, and relationship to function class capacity
- Understand that Linear Regression and l2-regularized linear regression have closed-form solutions (unlike most GLMs)
- Understand that this let's us characterize the bias and variance of these solutions
- Understand the LR solution is unbiased, if the true function is linear
- Understand LR+l2 is biased, but that asymptotically (as n grows) they reach the same solution
- Understand difference between realizable and nonrealizable settings
- **Will not be directly tested:**
  - Any specific closed-form solutions; I will give them to you if you need them

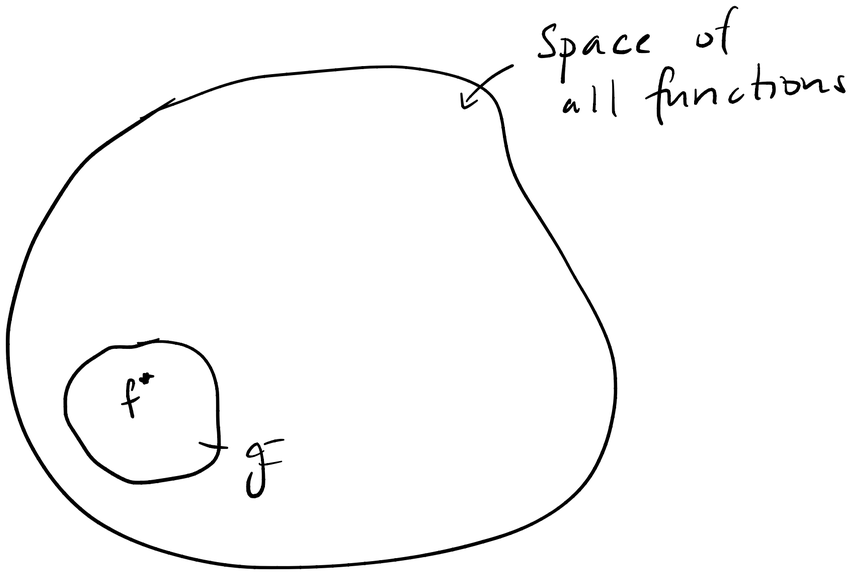
Ch4: Revisiting Generalization Error

- Understand that the generalization error of a function f is the error in expectation across all possible datapoints (expected cost)

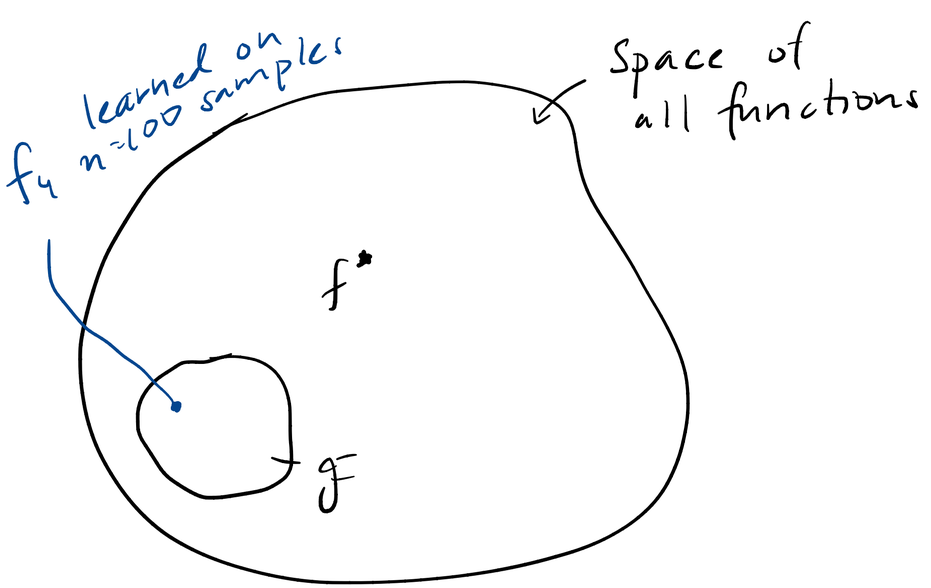
$$\mathrm{GE}(f) = \mathbb{E}[(f(X) - Y)^2] = \underbrace{\mathbb{E}[(f(X) - f^*(X))^2]}_{\text{reducible error}} + \underbrace{\mathbb{E}[(f^*(X) - Y)^2]}_{\text{irreducible error}}$$

- GE is about a specific function f, rather than about a function class where we have $f_{\mathscr{D}}$ that varies with data

Realizable vs Nonrealizable



(a) Realizable setting: $f^* \in \mathcal{F}$



(b) Non-realizable setting: $f^* \notin \mathcal{F}$

- For linear regression, assuming true f* uses the same features, we were able to directly compare learned w to w*. Is this the realizable or nonrealizable setting?

  $\mathbb{E}[\mathbf{w}(\mathscr{D})]$ compared to $\mathbf{w}^*$

- What is the definition for an estimator being unbiased more generally, if we do not compare weights?

Recall bias-variance for a function class

- Understand that we can reason about function $f_{\mathscr{D}}$ as a random variable, where randomness comes from the underlying dataset
- Understand that we can reason about expected generalization error (across datasets) of a function class, by considering the bias and variance of this $f_{\mathscr{D}}$
- Understand that reducible error of $f_{\mathscr{D}}$ decomposes into bias and variance
- For a specific x, we have

$$\mathbb{E}\left[\left(f_{\mathcal{D}}(\mathbf{x}) - f^*(\mathbf{x})\right)^2\right] = \left(\mathbb{E}\left[f_{\mathcal{D}}(\mathbf{x})\right] - f^*(\mathbf{x})\right)^2 + \mathrm{Var}\left[f_{\mathcal{D}}(\mathbf{x})\right]$$

Exercise: bias-variance across x

- For a specific x, we have

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- What is the bias-variance definition across all x?

Exercise: bias-variance across x

- For a specific x, we have

$$\mathbb{E}\left[(f_{\mathcal{D}}(\mathbf{x}) - f^*(\mathbf{x}))^2\right] = (\mathbb{E}\left[f_{\mathcal{D}}(\mathbf{x})\right] - f^*(\mathbf{x}))^2 + \mathrm{Var}\left[f_{\mathcal{D}}(\mathbf{x})\right]$$

- What is the bias-variance definition across all x?
  - Take expectation across the possible, from the data distribution
  - $p(\mathbf{x}, y) = p(y \,|\, \mathbf{x})p(\mathbf{x})$ so sample $\mathbf{x}$ from $p(\mathbf{x})$ for this expectation

$$\mathbb{E}[(f_{\mathcal{D}}(\boldsymbol{X}) - f^*(\boldsymbol{X}))^2] = \mathbb{E}_{\boldsymbol{X}}\left[(\mathbb{E}_{\mathcal{D}}[f_{\mathcal{D}}(\boldsymbol{X})] - f^*(\boldsymbol{X}))^2 + \mathrm{Var}_{\mathcal{D}}[f_{\mathcal{D}}(\boldsymbol{X})]\right]$$

Exercise

- Imagine we are in the realizable setting and the true function is linear. We know our MLE estimator (regular old linear regresion) is an unbiased estimator
- This means $\mathbb{E}[\mathbf{w}(\mathscr{D})] = \mathbf{w}^*$. Does this mean that $\mathbb{E}[f_{\mathbf{w}(\mathscr{D})}(\mathbf{x})] = f_{\mathbf{w}^*}(\mathbf{x})$?
  Recall that $f_{\mathbf{w}^*}(\mathbf{x}) = \boldsymbol{\phi}(\mathbf{x})\mathbf{w}^*$

Exercise

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- This means $\mathbb{E}[\mathbf{w}(\mathscr{D})] = \mathbf{w}^*$. Does this mean that $\mathbb{E}[f_{\mathbf{w}(\mathscr{D})}(\mathbf{x})] = f_{\mathbf{w}^*}(\mathbf{x})$? Recall that $f_{\mathbf{w}^*}(\mathbf{x}) = \boldsymbol{\phi}(\mathbf{x})\mathbf{w}^*$
- Ans: Yes. Notice $\mathbb{E}[f_{\mathbf{w}(\mathscr{D})}(\mathbf{x})] = \mathbb{E}[\boldsymbol{\phi}(\mathbf{x})\mathbf{w}(\mathscr{D})] = \boldsymbol{\phi}(\mathbf{x})\mathbb{E}[\mathbf{w}(\mathscr{D})] = \boldsymbol{\phi}(\mathbf{x})\mathbf{w}^*$

Discussion

- Why did we talk about bias-variance by comparing the weights, when we could have just always talked about the bias-variance for the functions?
- Why do we talk about bias-variance at all? Ultimately, we just care about how good our model is?
- Any other questions about GE and bias-variance?

Ch. 5: Optimization

- Understanding why the Hessian in the second-order update accounts for differences in curvature in different dimensions
- The mini-batch stochastic gradient descent (SGD) update rule
- Understanding why SGD is a more computationally efficient update than GD
- Understanding the importance of an adaptive vector stepsize, and that RMSProp and Adam use vector stepsizes
- Understanding the momentum update, used in Adam
- **Will not directly test**
  - Computing any weights, Hessians, etc., convergence theory and directional derivatives, knowing any of specific formulas (e.g, Adam, RMSProp, etc)

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 $c(\mathbf{w}) = \frac{1}{2}\|\mathbf{\Phi w} - \mathbf{y}\|_2^2 + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$. Is this mismatch a problem?
- How do we write the Ridge Regression loss as $c(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n} c_i(\mathbf{w})$?

A normalized RR objective

- $\frac{1}{2n}\sum_{i=1}^{n}(\boldsymbol{\phi}(\mathbf{x})_i\mathbf{w}-\mathbf{y}_i)^2+\frac{\lambda}{2n}\|\mathbf{w}\|_2^2$. What is ci?
- $c_i(\mathbf{w})=\frac{1}{2}(\boldsymbol{\phi}_i\mathbf{w}-y_i)^2+\frac{\lambda}{2n}\|\mathbf{w}\|_2^2$ because
- $\frac{1}{n}\sum_{i=1}^{n}\frac{1}{2}((\boldsymbol{\phi}(\mathbf{x})_i\mathbf{w}-\mathbf{y}_i)^2+\frac{\lambda}{2n}\|\mathbf{w}\|_2^2)=\frac{1}{2n}\sum_{i=1}^{n}(\boldsymbol{\phi}(\mathbf{x})_i\mathbf{w}-\mathbf{y}_i)^2+\frac{1}{n}\sum_{i=1}^{n}\frac{\lambda}{2n}\|\mathbf{w}\|_2^2$ and $\frac{1}{n}\sum_{i=1}^{n}\frac{\lambda}{2n}\|\mathbf{w}\|_2^2=\frac{1}{n}n\frac{\lambda}{2n}\|\mathbf{w}\|_2^2=\frac{\lambda}{2n}\|\mathbf{w}\|_2^2$
- Makes very clear that regularizer has a diminishing role with increasing n

A normalized RR objective

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

Why do we normalize the mini-batch by 1/b? We could absorb into stepsize? Any advantages to using 1/b to get the averaged stochastic gradient?

Exercise Question

- How might the size of the dataset n interact with the number of epochs that we need to converge?

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- How might the size of the dataset n interact with the number of epochs that we need to converge?
- **Answer**: With a very large dataset, we are doing more updates in each epoch and likely need fewer epochs to converge.

Chapter 6: GLMs

- Understand that Generalized Linear Models (GLMs) allow us to model
  - $p(y \mid \mathbf{x})$ = any natural exponential family distribution with natural parameter $\boldsymbol{\phi}(\mathbf{x})\mathbf{w}$
  - with associated transfer function g such that $g(\boldsymbol{\phi}(\mathbf{x})\mathbf{w})$ approximates $\mathbb{E}[Y \mid \mathbf{x}]$
- Know that linear regression, Poisson regression, logistic regression and multinomial logistic regression are examples of GLMs and their corresponding transfers
- Know that the GLM objectives are convex
- **Will not be directly tested:**
  - Knowing specific GLM updates; if I need you to reason about one I will give it to you
  - The details of exponential family distributions (5.2)

Exercise Question

- Imagine you have multinomial logistic regression implemented. How would you use this code to do binary classification?

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- Imagine you have multinomial logistic regression implemented. How would you use this code to do binary classification?
- Transform dataset of (x,y) with y in {0,1} or y in {-1,1} to dataset with y in {[1,0], [0,1]}, then call multinonimal logistic regression on this

Exercise Question

- Imagine we want to predict targets $y \in \{0,1,2,3,\ldots,20\}$
- What GLM could we use?

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- Imagine we want to predict targets $y \in \{0,1,2,3,\ldots,20\}$
- What GLM could we use?
  - The targets are ordered, so using Poisson regression would be sensible. When actually deploying, if the model predicted > 20, then would return 20
  - Could also use multinomial logistic regression, but this will just discard the potentially useful ordering to the data. (Why does this matter?)

Exercise Question

- Imagine we use a nonlinear transformation $\boldsymbol{\phi}(\mathbf{x})$ using RBF features
- We run SGD with large minibatches for millions of epochs on the Poisson regression loss, until convergence (very small gradients)
- Can we guarantee we are at a global minima, or could we be stuck in a local minima or saddlepoint?

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- What if instead we learned a nonlinear transformation on $\mathbf{x}$ using a neural network, again with the Poisson regression loss for millions of epochs?

Exercise Question

- Imagine we use a nonlinear transformation $\boldsymbol{\phi}(\mathbf{x})$ using RBF features
- Can we guarantee we are at a global minima, or could we be stuck in a local minima or saddlepoint?
  - **Ans**: Our Poisson regression objective is convex, for a fixed representation, even though the prediction itself is nonlinear in $\mathbf{x}$ due to using $\boldsymbol{\phi}(\mathbf{x})$
- What if instead we learned a nonlinear transformation on $\mathbf{x}$ using a neural network, again with the Poisson regression loss for millions of epochs?
  - **Ans**: The objective is no longer convex, cannot guarantee global min

Exercise Question

- What is instead we 1) initialize weights randomly in the NN and 2) freeze all the weights in the layers except the output layer, $\mathbf{W}^{(1)}$
- For a given input $\mathbf{x}$, we pass through multiple fixed layers to get to the final layer $\mathbf{h}^{(1)}$ and make prediction $\exp(\mathbf{h}^{(1)}\mathbf{W}^{(1)})$
- Imagine we train $\mathbf{W}^{(1)}$ for millions of epochs with the Poisson regression loss. Can we guarantee we are at a global minima, or could we be stuck in a local minima or saddlepoint?

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- Imagine we train $\mathbf{W}^{(1)}$ for millions of epochs with the Poisson regression loss. Can we guarantee we are at a global minima, or could we be stuck in a local minima or saddlepoint?
  - **Ans**: Yes. The network just provides another fixed representation $\boldsymbol{\phi}(\mathbf{x}) \doteq \mathbf{h}^{(1)}$, (loss if convex for that last layer)

Exercise Question

- Imagine we use a nonlinear transformation $\boldsymbol{\phi}(\mathbf{x})$ using RBF features
- We run SGD with large minibatches for millions of epochs on the Poisson regression loss, **but now we also add l2 regularization.**
- Can we guarantee we are at a global minima, or could we be stuck in a local minima or saddlepoint?

Exercise Question

- Imagine we use a nonlinear transformation $\boldsymbol{\phi}(\mathbf{x})$ using RBF features
- We run SGD with large minibatches for millions of epochs on the Poisson regression loss, but now we also add l2 regularization.
- Can we guarantee we are at a global minima, or could we be stuck in a local minima or saddlepoint?
  - **Ans**: Yes. The l2 regularizer is convex in the weights, and the sum of two convex functions is again convex

Chapter 7: Constrained Optimization

- Optimization of the form $\min_{\mathbf{w} \in \mathbb{R}^p} c(\mathbf{w}) + r(\mathbf{w})$ for smooth c, nonsmooth r
- Understand need to use a different approach due to nonsmooth r, including for constrained optimization
- Proximal update: $\mathbf{w}_{t+1} = \text{prox}_{\eta_t r}(\mathbf{w}_t - \eta_t \nabla c(\mathbf{w}_t))$
- That we use proximal GD with l1 regularization, and that l1 regularization on the weights encourages weights to be zero
- **Will not test**
  - Specific proximal operators
  - Vector stepsizes or momentum with proximal operators; we only did scalar stepsizes
  - I will not get you to derive solutions with Lagrangians (Section 7.3)

Proximal operators

- Optimize with smooth $c(\mathbf{w})$ and non-smooth $r(\mathbf{w})$
- To solve $\min_{\mathbf{w}\in\mathbb{R}^d} c(\mathbf{w}) + r(\mathbf{w})$ we break it into two steps
- GD Step: $\tilde{\mathbf{w}}_{t+1} = \mathbf{w}_t - \eta \nabla c(\mathbf{w}_t)$
- Projection step: $\mathbf{w}_{t+1} = \text{prox}_{\eta r}(\tilde{\mathbf{w}}_{t+1})$ where the proximal operator is
- $\text{prox}_{\eta r}(\mathbf{u}) = \arg\min_{\mathbf{w}\in\mathbb{R}^d} \frac{1}{2}\|\mathbf{w} - \mathbf{u}\|_2^2 + \eta r(\mathbf{w})$

Simple example of a proximal operator

- You solved for $\text{prox}_{\eta r}(\mathbf{u}) = \arg\min_{\mathbf{w}\in\mathbb{R}^d} \frac{1}{2}\|\mathbf{w}-\mathbf{u}\|_2^2 + \eta r(\mathbf{w})$ for $r(\mathbf{w}) = \lambda\|\mathbf{w}\|_1$
- Let's do another simple example with $r(\mathbf{w}) = \frac{\lambda}{2}\|\mathbf{w}\|_2$
- Not necessary to use proximal gradient descent for this regularizer, because it is smooth, so it can just be included in c. But, we can if we want
- **Note**: we cannot do the other way. We cannot take nonsmooth parts and just include them in c, because we must be able to take the gradient of c for the first part of the proximal update

Proximal operator for l2-regularization

- $\text{prox}_{\eta_t \frac{\lambda}{2} \ell_2}(\tilde{\mathbf{w}}_{t+1}) = \arg\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{2}\|\mathbf{w} - \tilde{\mathbf{w}}_{t+1}\|_2^2 + \eta_t \lambda \frac{1}{2}\|\mathbf{w}\|_2^2$
- Closed-form solution is given by
- $\nabla \left(\frac{1}{2}\|\mathbf{w} - \tilde{\mathbf{w}}_{t+1}\|_2^2 + \eta_t \lambda \frac{1}{2}\|\mathbf{w}\|_2^2 \right) = \mathbf{w} - \tilde{\mathbf{w}}_{t+1} + \eta_t \lambda \mathbf{w} = 0$
- Implies $\mathbf{w} = (1 + \eta_t \lambda)^{-1} \tilde{\mathbf{w}}_{t+1} = (1 + \eta_t \lambda)^{-1} (\mathbf{w}_t - \eta_t \nabla c(\mathbf{w}_t))$
- Self-test: What exactly is $\text{prox}_{\eta_t \frac{\lambda}{2} \ell_2}(\tilde{\mathbf{w}}_{t+1})$ here?

Chapter 8: Cross Validation

- Understand that cross validation allows us to estimate GE of a model trained on the entire dataset, without having to have a hold-out test set
- Understand the k-fold CV algorithm
- Understand the repeated random subsampling (RRS) CV algorithm
- General role k and p play in the bias of our GE estimator (outlined in these slides)
- **Will not test**
  - The more detailed nuances about the bias-variance distinctions for different CV choices

Chapter 8: Cross Validation

- Know what it means to select hyperparameters
- Understand the utility of CV for hyperparameter selection
- Understand the difference between internal CV and external CV in nested CV
  - internal CV is for hyperparameter selection and external is to evaluate the algorithm that might use internal CV
- **Will not be directly tested:**
  - Knowing how to pick the set of hyperparameters to be tested with CV

Exercise Question

Do we have to use nested cross-validation?

- When should we use a single train-validation-test split?

Exercise Question

Do we have to use nested cross-validation?

- When should we use a single train-validation-test split?
  - We have a massive dataset, so can make train, validation and test big
  - And sometimes compromise if our model is very expensive to train, making CV impractical to use

Exercise Question

Do we have to use nested cross-validation?

- When should we use a single train-validation-test split?
- Why does CV only have train and test partitions? Why aren’t there also three datasets (train, validation and test)?

Exercise Question

Do we have to use nested cross-validation?

- When should we use a single train-validation-test split?
- Why does CV only have train and test partitions? Why aren’t there also three datasets (train, validation and test)?
  - Validation is used for hyperparameter selection (role of internal CV)
  - Test is used for evaluation of the final function (role of external CV)
  - CV uses the whole dataset for both evaluation and training, so it actually only makes splits for evaluation, and trains on the entire dataset

Exercise Question

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- When should we use a single train-validation-test split?
- Why does CV only have train and test partitions? Why aren’t there also three datasets (train, validation and test)?
- Do we have to use nested cross validation? Can we use a single train-test split externally, and k-fold CV internally?

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- Do we have to use nested cross validation? Can we use a single train-test split externally, and k-fold CV internally?
  - Yes! The learner uses CV to algorithmically set its hyperparameters. We can evaluate this learner in any way we want (external CV or one train-test split)

Exercise Question

Do we have to use nested cross-validation?

- When should we use a single train-validation-test split?
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- Can we use a single train-validation split internally, and CV externally?

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- Why does CV only have train and test partitions? Why aren't there also three datasets (train, validation and test)?
- Do we have to use nested cross validation? Can we use a single train-test split externally, and k-fold CV internally?
- Can we use a single train-validation split internally, and CV externally?
  - Yes! The learner uses a validation set to algorithmically set its hyperparameters. We can evaluate this learner in any way we want.

Exercise Question

Do we have to use nested cross-validation?

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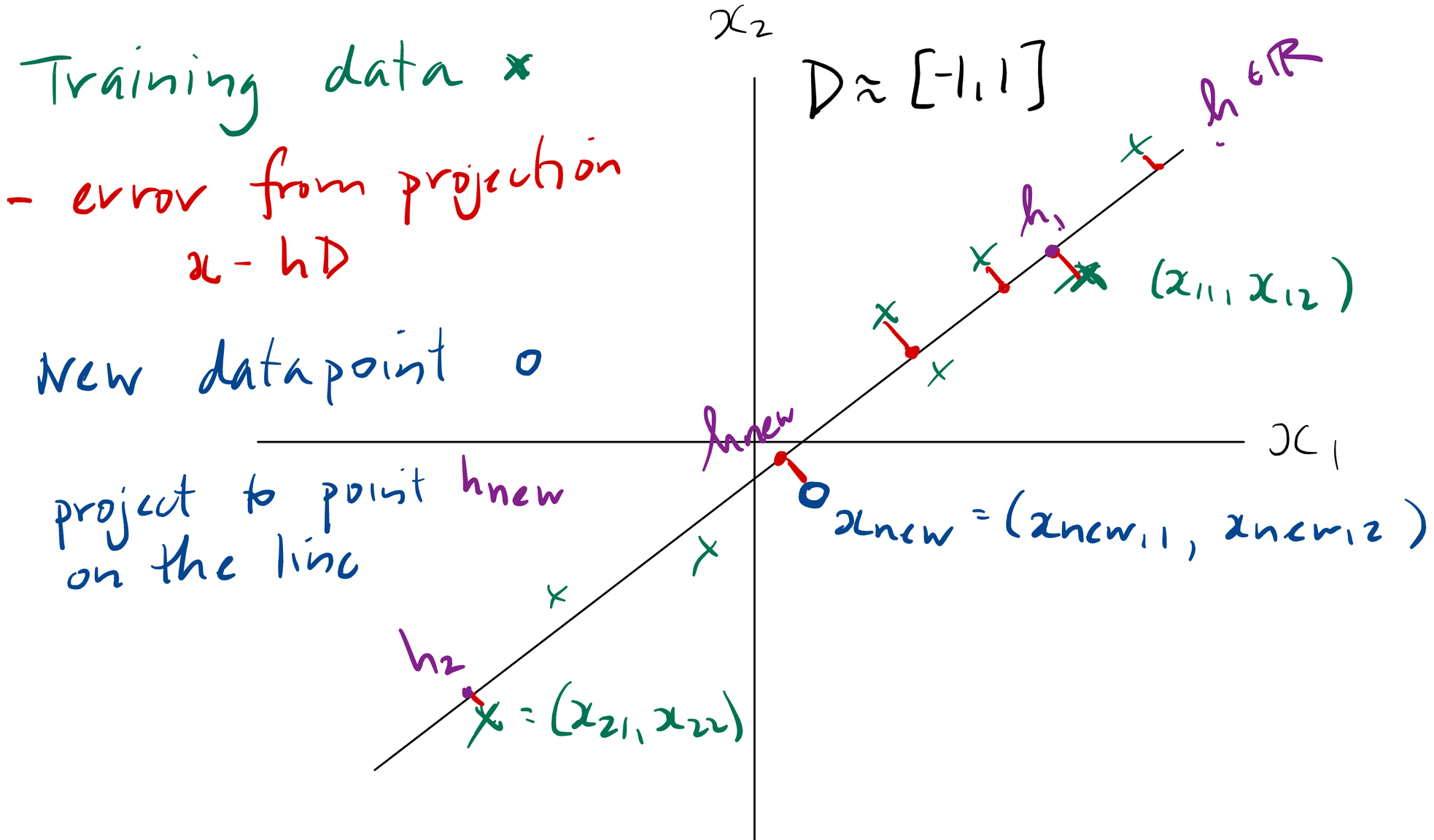
- Why does CV only have train and test partitions? Why aren’t there also three datasets (train, validation and test)?
- Do we have to use nested cross validation? Can we use a single train-test split externally, and k-fold CV internally?
- Can we use a single train-validation split internally, and CV externally?
- Should we do either of these?

Chapter 9: Latent Factors

- Understand that PCA extracts a lower-dimensional representation
- Understand the objective underlying PCA (minimize $\|\mathbf{x} - \mathbf{hD}\|_2^2$ for every x)
- Understand that sparse coding similarly minimizes $\|\mathbf{x} - \mathbf{hD}\|_2^2$, but additionally has an l1 regularizer on h to find a high-dimensional sparse representation
- **Will not be directly tested:**
  - PPCA
  - Algorithms for PCA and sparse coding
  - Interpretations of latent factors (was only for intuition about what might be learned)

PCA on training data and new points



Exercise Question

- Imagine we first expand the dimension using a kernel representation, going from 10 features to 5000.
- Imagine we compute the SVD of Phi, and the top 100 singular values are reasonably big, and the rest are relatively small.
- We decide to use PCA to get 100 features (i.e., use the computed SVD and take the top k singular vectors as the new representation).
- How do we interpret these 100 features?

Chapter 10: Neural Networks

- Understand transformation on the input given by a simple feedforward neural network
  - series of linear functions composed with simple activations
- Understand that backpropagation is gradient descent
- Understand can use different architectures: skip connections, convolutions, sparse connectivity
- **Will not test**
  - You will not need to derive gradients for an NN, nor know the backprop update formulas

Exercise Question

- We discussed that many transformations consist of (1) linear weighting followed by (2) nonlinear activation (differentiable almost everywhere)
- What are some other activations we could consider using in a network, beyond the three we discussed (ReLU, sigmoid, tanh)? Why would these be reasonable?

Exercise Question

Assume we are predicting a scalar target

- Write down the set of functions $\mathscr{F}_1$ obtained using a kernel representation with kernel k, and a random subset of 100 points from the training data as centers, giving features $\boldsymbol{\phi}(\mathbf{x}) \in \mathbb{R}^{101}$ (assume $\mathscr{X}$ space of possible inputs $\mathbf{x}$)

- Write down the set of functions $\mathscr{F}_2$ obtained using an NN with one hidden layers of size 256, with ReLu activations, for regression

Exercise Question

Assume we are predicting a scalar target

- Write down the set of functions $\mathcal{F}_1$ obtained using a kernel representation with kernel k, and a random subset of 100 points from the training data as centers, giving features $\boldsymbol{\phi}(\mathbf{x}) \in \mathbb{R}^{101}$ (assume $\mathcal{X}$ space of possible inputs $\mathbf{x}$)
  - Ans: $\mathcal{F}_1 = \{f : \mathcal{X} \to \mathbb{R} : f(\mathbf{x}) = \boldsymbol{\phi}(\mathbf{x})\mathbf{w}$ for any $\mathbf{w} \in \mathbb{R}^{101}\}$
- Write down the set of functions $\mathcal{F}_2$ obtained using an NN with one hidden layers of size 256, with ReLu activations, for regression
  - Ans:
    $\mathcal{F}_2 = \{f : \mathcal{X} \to \mathbb{R} : f(\mathbf{x}) = \text{ReLU}(\mathbf{x}\mathbf{W}^{(2)})\mathbf{W}^{(1)}$ for any $\mathbf{W}^{(1)} \in \mathbb{R}^{256\times 1}, \mathbf{W}^{(2)} \in \mathbb{R}^{d\times 256}\}$

Exercise Question

- Write down the set of functions $\mathscr{F}_1$ obtained using a kernel representation with kernel k, and a random subset of 100 points from the training data as centers, giving features $\boldsymbol{\phi}(\mathbf{x}) \in \mathbb{R}^{101}$ (assume $\mathscr{X}$ space of possible inputs $\mathbf{x}$)
- Write down the set of functions $\mathscr{F}_2$ obtained using an NN with one hidden layers of size 256, with ReLu activations, for regression
- If I told you that an $\mathscr{F}_1$ is a subset of $\mathscr{F}_2$, what does that mean? Which class has higher complexity (or capacity)?
- How do you know one is a subset of the other? Is $\mathscr{F}_1$ a subset of $\mathscr{F}_2$ here?

Exercise Question

- Recall bias-variance decomposition

$$\mathbb{E}\left[(f_{\mathcal{D}}(\mathbf{x}) - f^*(\mathbf{x}))^2\right] = (\mathbb{E}\left[f_{\mathcal{D}}(\mathbf{x})\right] - f^*(\mathbf{x}))^2 + \mathrm{Var}\left[f_{\mathcal{D}}(\mathbf{x})\right]$$

- Imagine $\mathscr{F}_1$ is a subset of $\mathscr{F}_2$
- Do you think $\mathscr{F}_1$ or $\mathscr{F}_2$ has higher bias?
- Do you think $\mathscr{F}_1$ or $\mathscr{F}_2$ has higher variance?

Exercise Question

- Recall bias-variance decomposition

$$\mathbb{E}\left[\left(f_{\mathcal{D}}(\mathbf{x}) - f^*(\mathbf{x})\right)^2\right] = \left(\mathbb{E}\left[f_{\mathcal{D}}(\mathbf{x})\right] - f^*(\mathbf{x})\right)^2 + \mathrm{Var}\left[f_{\mathcal{D}}(\mathbf{x})\right]$$

- Imagine $\mathscr{F}_1$ is a subset of $\mathscr{F}_2$
- Do you think $\mathscr{F}_1$ or $\mathscr{F}_2$ has higher bias? **Ans**: Yes, equal or higher bias
- Do you think $\mathscr{F}_1$ or $\mathscr{F}_2$ has higher variance? **Ans**: No, equal or lower variance

Chapter 11: Regularization for NNs

- Understand that linear autoencoders also extract a low-dimensional representation like PCA
- Understand we can use the reconstruction loss as an auxiliary loss
- **Will not be directly tested:**
  - Good to know about the ability to use auxiliary losses, but will not be directly tested on supervised autoencoders
  - Will not be tested on Section 11.3 (double descent)

Exercise

- We saw a linear autoencoder is equivalent to PCA
  - $f_{\mathbf{w}}(\mathbf{x}) = \mathbf{x}\mathbf{W}^{(2)}\mathbf{W}^{(1)}$ with bottleneck ($\mathbf{W}^{(2)} \in \mathbb{R}^{d \times k}, \mathbf{W}^{(1)} \in \mathbb{R}^{k \times d}, k < d$
- What if we use a multilayer autoencoder with nonlinear activations?
  - $f_{\mathbf{w}}(\mathbf{x}) = f_1(f_2(f_3(\mathbf{x}\mathbf{W}^{(3)})\mathbf{W}^{(2)})\mathbf{W}^{(1)})$
- What is the size of the output, $f_{\mathbf{w}}(\mathbf{x})$?
- What loss do we use to train this multilayer autoencoder?

Exercise

- We saw a linear autoencoder is equivalent to PCA
- What if we use a multilayer autoencoder with nonlinear activations
  - $f_{\mathbf{w}}(\mathbf{x}) = f_1(f_2(f_3(\mathbf{x}\mathbf{W}^{(3)})\mathbf{W}^{(2)})\mathbf{W}^{(1)})$
- What is the size of the output, $f_{\mathbf{w}}(\mathbf{x})$?
  - **Ans**: Same size as $\mathbf{x}$, because we are trying to reconstruct $\mathbf{x}$
- What loss do we use to train this multilayer autoencoder?
  - **Ans**: Reconstruction error to $\mathbf{x}$ (e.g., squared-error loss $\|\mathbf{x} - \hat{\mathbf{x}}\|_2^2$)

Chapter 12: Mixture Models

- Understand how we sample from mixture models
- Understand that the EM algorithm consists of (a) the introduction of auxiliary variables z (which component of the mixture a sample belongs to) and (b) alternating between updating $p(z_i \mid \mathbf{x}_i)$ and parameters $\mathbf{w}$
- Understand that the E-step updates $p(z_i \mid \mathbf{x}_i)$ for fixed $\mathbf{w}$, and the M-step updates $\mathbf{w}$ for fixed $p(z_i \mid \mathbf{x}_i)$ with each component updated independently using a (weighted) log-likelihood
- **Will not be directly tested:**
  - You do not need to memorize the EM algorithm, but you should be able to recognize key components of it

EM Algorithm for any component distribution

$\mathbf{w} = (\boldsymbol{\theta}, \boldsymbol{\alpha})$

Algorithm 10: EM for any component distribution

Input: number of components m, with components distributions $p(\cdot|\boldsymbol{\theta}_1), \ldots, p(\cdot|\boldsymbol{\theta}_m)$

Initialize $\theta_k^{(0)}$ and $\alpha_k^{(0)}$ for all $k \in 1$ to m, $t = 0$

while not converged **do**

  $p_t[i,k] = \frac{\alpha_k^{(t)} p(\mathbf{x}_i|\boldsymbol{\theta}_k^{(t)})}{\sum_{j=1}^m \alpha_j^{(t)} p(\mathbf{x}_i|\boldsymbol{\theta}_j^{(t)})}$ for all $i \in \{1,2,\ldots,n\}$, $k \in \{1,2,\ldots,m\}$

  Compute $p_t[k] \stackrel{\text{def}}{=} \frac{1}{n} \sum_{i=1}^n p_t[i,k]$

  for $k \in \{1,2,\ldots,m\}$ **do**

    $\alpha_k^{(t+1)} = p_t[k]$

    $\boldsymbol{\theta}_k^{(t+1)} = \text{argmin}_{\boldsymbol{\theta}_k} - \sum_{i=1}^n p_t[i,k] \ln p(\mathbf{x}_i|\boldsymbol{\theta}_k)$

  $t \leftarrow t+1$

return $\alpha_k^t, \boldsymbol{\theta}_k^{(t)}$ for all $k \in \{1,2,\ldots,m\}$

Which part is the E step (update $p(z_i \mid \mathbf{x}_i)$) and which is the M step (update $\mathbf{w}$)?

EM Algorithm for any component distribution

$\mathbf{w} = (\boldsymbol{\theta}, \boldsymbol{\alpha})$

Algorithm 10: EM for any component distribution

Input: number of components m, with components distributions $p(\cdot|\boldsymbol{\theta}_1), \ldots, p(\cdot|\boldsymbol{\theta}_m)$

Initialize $\theta_k^{(0)}$ and $\alpha_k^{(0)}$ for all $k \in 1$ to m, $t = 0$

while not converged **do**

E-step

$$p_t[i,k] = \frac{\alpha_k^{(t)} p(\mathbf{x}_i|\boldsymbol{\theta}_k^{(t)})}{\sum_{j=1}^{m} \alpha_j^{(t)} p(\mathbf{x}_i|\boldsymbol{\theta}_j^{(t)})} \text{ for all } i \in \{1,2,\ldots,n\},\ k \in \{1,2,\ldots,m\}$$

Compute $p_t[k] \stackrel{\text{def}}{=} \frac{1}{n} \sum_{i=1}^{n} p_t[i,k]$

for $k \in \{1,2,\ldots,m\}$ **do**

M-step

$$\alpha_k^{(t+1)} = p_t[k]$$

$$\boldsymbol{\theta}_k^{(t+1)} = \text{argmin}_{\boldsymbol{\theta}_k} - \sum_{i=1}^{n} p_t[i,k] \ln p(\mathbf{x}_i|\boldsymbol{\theta}_k)$$

$t \leftarrow t + 1$

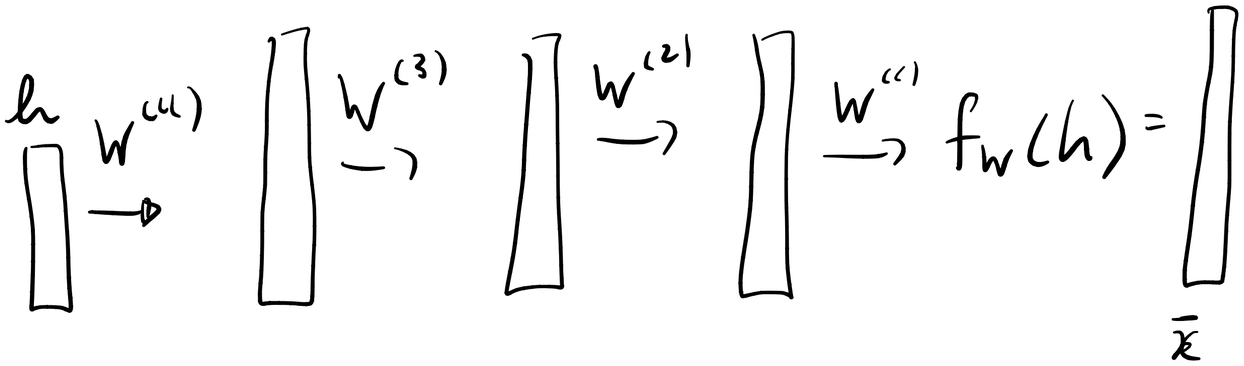
return $\alpha_k^t, \boldsymbol{\theta}_k^{(t)}$ for all $k \in \{1,2,\ldots,m\}$

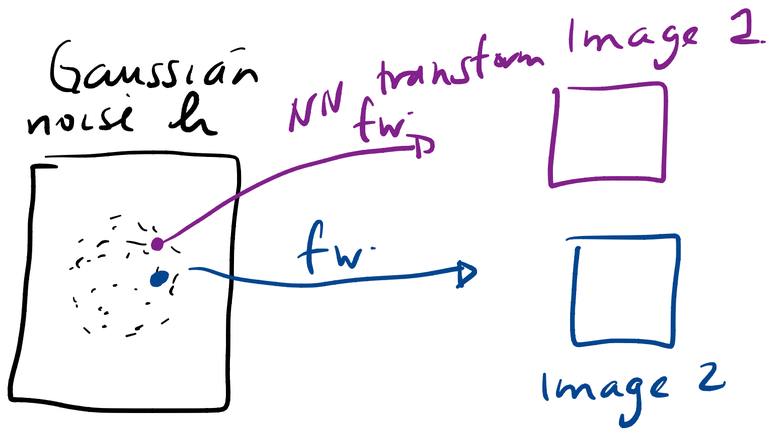
Which part is the E step (update $p(z_i \mid \mathbf{x}_i)$) and which is the M step (update $\mathbf{w}$)?

Chapter 13: Generative Models using Data Reps

- Understand that both PPCA and VAEs make the assumption that
- $p(\mathbf{x}) = \int p(\mathbf{x}\,|\,\mathbf{h})p(\mathbf{h})d\mathbf{h}$ with $p(\mathbf{h}) = \mathcal{N}(\mathbf{0}, \mathbf{I})$
- Understand that PPCA assumes a linear relationship between $\mathbf{x}$ and $\mathbf{h}$
  $p(\mathbf{x}\,|\,\mathbf{h}) = \mathcal{N}(\mathbf{hD}, \sigma^2\mathbf{I})$
- And that VAE generalizes to a nonlinear relationship, using NN $f_{\mathbf{W}}$ to give
  $p(\mathbf{x}\,|\,\mathbf{h}) = \mathcal{N}(f_{\mathbf{W}}(\mathbf{h}), \sigma^2\mathbf{I})$
- Understand how to sample from a VAE
  - Step 1: Sample $\mathbf{h} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ and then
  - Step 2: Return $f_{\mathbf{W}}(\mathbf{h})$ (where $f_{\mathbf{W}}$ is the decoder part of the network)

Visualizing this function





- VAE generalizes to a nonlinear relationship, using NN $f_{\mathbf{W}}$ to give $p(\mathbf{x} \mid \mathbf{h}) = \mathcal{N}(f_{\mathbf{W}}(\mathbf{h}), \sigma^2 \mathbf{I})$
- Understand how to sample from a VAE
  - Step 1: Sample $\mathbf{h} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ and then
  - Step 2: Return $f_{\mathbf{W}}(\mathbf{h})$ or sample $\mathbf{x} \sim \mathcal{N}(f_{\mathbf{W}}(\mathbf{h}), \sigma^2 \mathbf{I})$

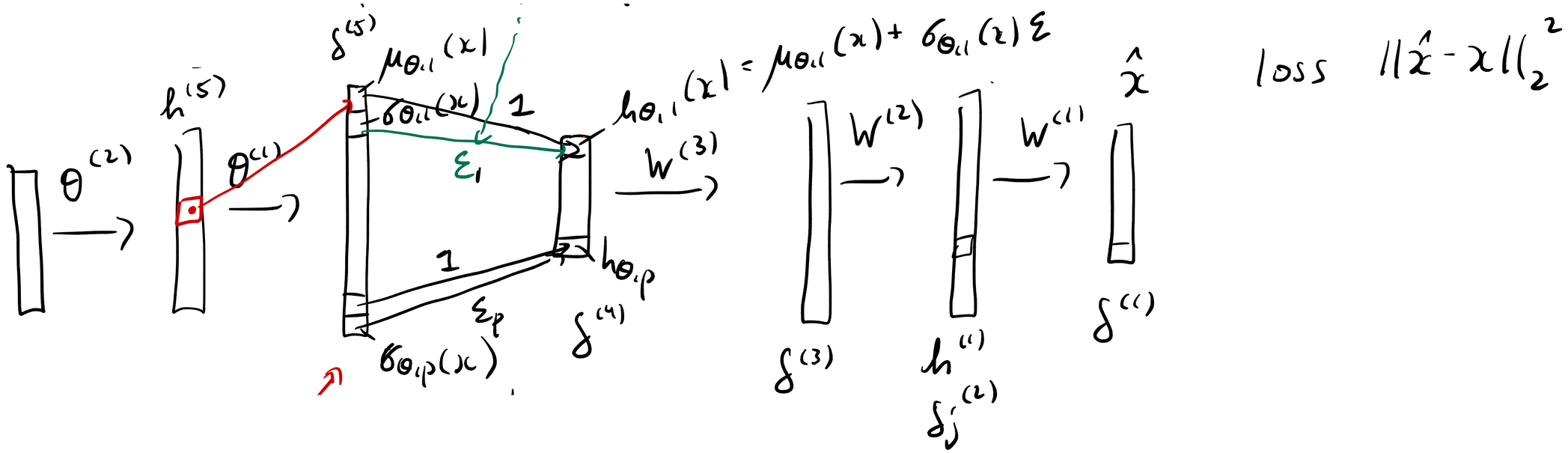
Chapter 12: VAEs (cont)

- Understand our goal is to minimize $\sum_{i=1}^{n} -\ln p(\mathbf{x}_i \,|\, \mathbf{W})$
  - But that this is hard to because $p(\mathbf{x}_i \,|\, \mathbf{W})$ involves an integral over hidden $\mathbf{h}$
- Understand that we learn the encoder $q(\mathbf{h} \,|\, \mathbf{x})$ only as part of the optimization, to help us learn $p(\mathbf{x} \,|\, \mathbf{h})$; we do not need $q(\mathbf{h} \,|\, \mathbf{x})$ itself for deployment
- Understand that we derive the VAE objective by starting with $-\ln p(\mathbf{x} \,|\, \mathbf{W}) + D_{KL}(q_\theta(\,\cdot\,|\,\mathbf{x}) \,||\, p(\,\cdot\,|\,\mathbf{x}, \mathbf{W}))$ and rearranging terms to get $D_{KL}(q_\theta(\,\cdot\,|\,\mathbf{x}) \,||\, \mathcal{N}(0, \mathbf{I})) - \mathbb{E}_{\mathbf{h} \sim q_\theta(\cdot|\mathbf{x})}[\ln p(\mathbf{x} \,|\, \mathbf{h}, \mathbf{W})]$ (the negative ELBO)

Discussion questions

- Why is our minimization $\min_{\mathbf{W},\boldsymbol{\theta}} -\ln p(\mathbf{x}\,|\,\mathbf{W}) + D_{KL}(q_\theta(\,\cdot\,|\,\mathbf{x})\,||\,p(\,\cdot\,|\,\mathbf{x},\mathbf{W}))$?
- (And why do we write $q_\theta(\,\cdot\,|\,\mathbf{x})$ instead of $q(\,\cdot\,|\,\mathbf{x},\theta)$?)
- Why is it equivalent to instead minimize the negative ELBO?
  $\min_{\mathbf{W},\boldsymbol{\theta}} D_{KL}(q(\,\cdot\,|\,\mathbf{x})\,||\,\mathcal{N}(0,\mathbf{I})) - \mathbb{E}_{\mathbf{h}\sim q(\cdot|\mathbf{x})}[\ln p(\mathbf{x}\,|\,\mathbf{h},\mathbf{W})]$
- How does this look if I maximize the ELBO?
- If we change $p(\mathbf{x}\,|\,\mathbf{h}) = \mathcal{N}(f_{\mathbf{W}}(\mathbf{h}), \sigma^2\mathbf{I})$ to $p(\mathbf{x}\,|\,\mathbf{h}) = \text{Bernoulli}(f_{\mathbf{W}}(\mathbf{h}))$, then do we also have to change the distribution $p(\mathbf{h}) = \mathcal{N}(\mathbf{0}, \mathbf{I})$?

Exercise: which part is q and p?



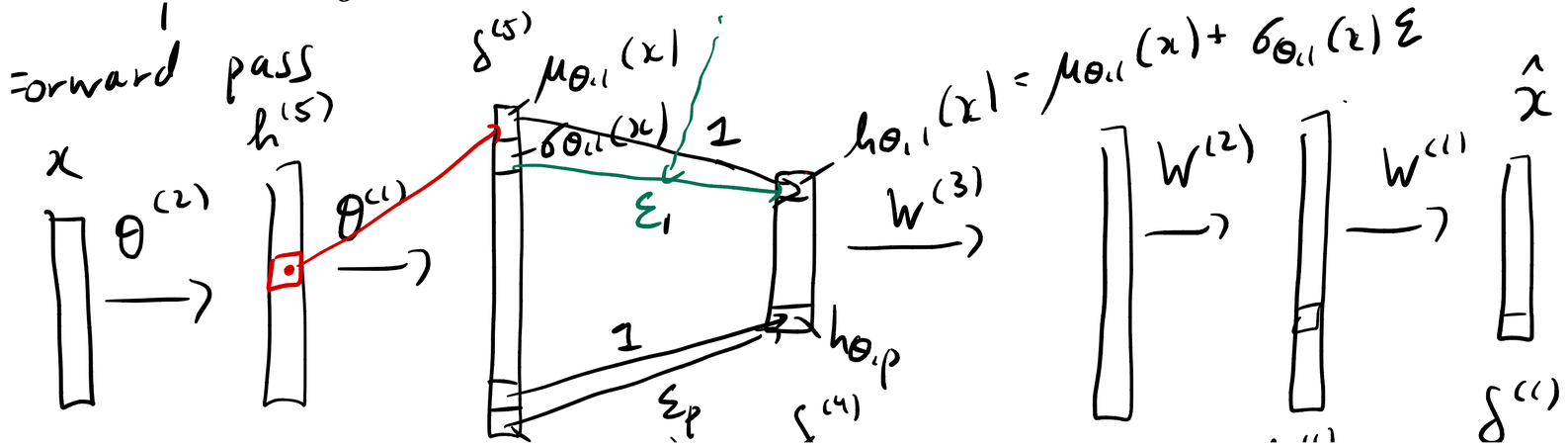
- Recall we parameterized our encoder as $q(\mathbf{h} \mid \mathbf{x}, \boldsymbol{\theta}) = \mathcal{N}(f_{\mu,\theta}(\mathbf{x}), f_{\sigma,\theta}(\mathbf{x}))$

Chapter 12: VAEs (cont)

- Understand our goal is to minimize $\sum_{i=1}^{n} -\ln p(\mathbf{x}_i \,|\, \mathbf{W})$
  - But that this is hard to because $p(\mathbf{x}_i \,|\, \mathbf{W})$ involves an integral over hidden $\mathbf{h}$
- Understand that we learn the encoder $q(\mathbf{h} \,|\, \mathbf{x})$ only as part of the optimization, to help us learn $p(\mathbf{x} \,|\, \mathbf{h})$; we do not need $q(\mathbf{h} \,|\, \mathbf{x})$ itself for deployment
- Understand that we derive the VAE objective by starting with $-\ln p(\mathbf{x} \,|\, \mathbf{W}) + D_{KL}(q_\theta(\,\cdot\,|\,\mathbf{x}) \,||\, p(\,\cdot\,|\,\mathbf{x}, \mathbf{W}))$ and rearranging terms to get $D_{KL}(q_\theta(\,\cdot\,|\,\mathbf{x}) \,||\, \mathcal{N}(0, \mathbf{I})) - \mathbb{E}_{\mathbf{h} \sim q_\theta(\cdot|\mathbf{x})}[\ln p(\mathbf{x} \,|\, \mathbf{h}, \mathbf{W})]$ (the negative ELBO)
- Understand why we use the reparameterization trick to get the gradient

Exercise: Reparameterization trick

- Recall we parameterized our encoder as $q(\mathbf{h} \mid \mathbf{x}, \boldsymbol{\theta}) = \mathcal{N}(f_{\mu,\theta}(\mathbf{x}), f_{\sigma,\theta}(\mathbf{x}))$
- We used reparameterization
  $\mathbb{E}_{\mathbf{h}\sim q(\cdot|\mathbf{x})}[\ln p(\mathbf{x} \mid \mathbf{h}, \mathbf{W})] = \mathbb{E}_{\boldsymbol{\epsilon}\sim\mathcal{N}(0,\mathbf{I})}[\ln p(\mathbf{x} \mid h_j = \mu_j(\mathbf{x}) + \sigma_j(\mathbf{x})\boldsymbol{\epsilon}_j, \mathbf{W})]$
- Q1: What is the dimension of $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$? How is this sampled?
- Q2: What if we decided we wanted discrete hidden h and used $q(\mathbf{h} \mid \mathbf{x}, \boldsymbol{\theta}) = \text{softmax}(f_\theta(\mathbf{x}))$? How does the NN change? Can we still use reparam?



Exercise: Reparameterization trick

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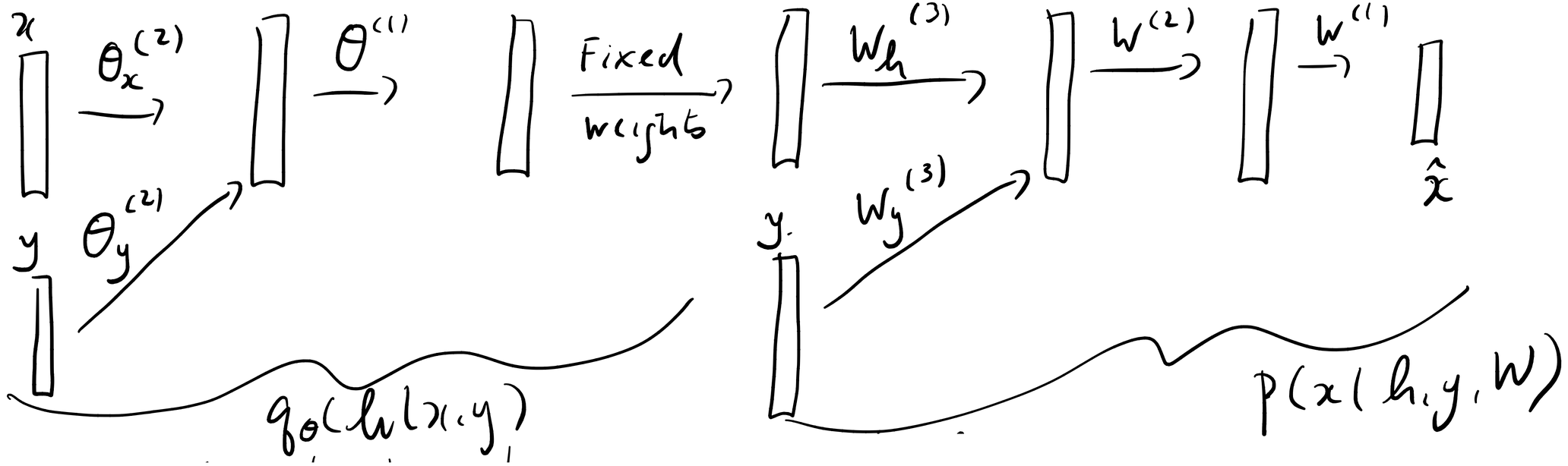
- We used reparameterization
  $\mathbb{E}_{\mathbf{h}\sim q(\cdot|\mathbf{x})}[\ln p(\mathbf{x} \mid \mathbf{h}, \mathbf{W})] = \mathbb{E}_{\boldsymbol{\epsilon}\sim\mathcal{N}(0,\mathbf{I})}[\ln p(\mathbf{x} \mid h_j = \mu_j(\mathbf{x}) + \sigma_j(\mathbf{x})\boldsymbol{\epsilon}_j, \mathbf{W})]$
- Q1: What is the dimension of $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$? How is this sampled?
  - **Ans**: size of h (size k), independently get k samples from a normal distribution $\mathcal{N}(0,1)$
- Q2: What if we decided we wanted discrete hidden h and used
  $q(\mathbf{h} \mid \mathbf{x}, \boldsymbol{\theta}) = \text{softmax}(f_\theta(\mathbf{x}))$? How does the NN change? Can we still use reparam?
  - **Ans**: If the number of discrete items is m (h in {1, 2, …, m}), the hidden dimension is k*m sized, i.e., softmax outputs repeated k times (one for each h1, …, hk that will be sampled)
  - It is not longer straightforward to use reparameterization

Exercise

- To sample from a VAE, we use
  - Step 1: Sample $\mathbf{h} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ and then
  - Step 2: query the decoder part of the VAE network $f_{\mathbf{W}}(\mathbf{h})$
- Why don't we sample $\mathbf{h}$ from $q(\mathbf{h} \mid \mathbf{x})$?

Chapter 13: Conditional VAEs



Chapter 13: VAEs (cont)

- **Will not be directly tested**
  - Memorizing the VAE objective (I will give you formulas)
  - Memorizing the gradient update for the VAE
  - The connection to Expectation-Maximization (9.3)
  - Deriving the gradient with the reparameterization trick

Chapter 13: Evaluating Generative Models

- Understand goal is to estimate $\hat{\text{GE}}(\boldsymbol{\theta}) = \frac{1}{m} \sum_{x_i \in \mathcal{D}_{\text{test}}} -\ln p(\mathbf{x}_i \mid \boldsymbol{\theta})$
- Understand that can easily compute this for a mixture model, as long as easy to compute $-\ln p(\mathbf{x}_i \mid \boldsymbol{\theta}_k)$ for each component
- Understand that this is hard to compute for VAEs, must be estimated, and that we again leveraged $q_\theta(\mathbf{h} \mid \mathbf{x})$ to do so
- **Will not be directly tested**
  - the exact importance sampling algorithm to estimate this GE for VAEs

Exercise

- How would you use k-fold CV to pick the number of centers for a Gaussian Mixture Model (GMM)?

Exercise

- How would you use k-fold CV to pick the number of centers for a Gaussian Mixture Model (GMM)?
- Answer: You would decide on the set of numbers to select from,
  e.g., H = {2, 4, 8, 16}
- After partitioning the data into k folds, for each hyper m in H and each fold f
  - Learn the GMM $\hat{p}$ on all but fold f
  - Evaluate on fold f, by computing the negative log likelihood on the data
    $$\sum_{x \in \text{fold f}} -\ln \hat{p}(x)$$

Exercise

- Can we take a mixture over VAE components?

Exercise

- Can we take a mixture over VAE components?
  - Yes! Not sure its useful, but seems fun. Go back to the MM algorithms and see if you can figure out how to do it by

Algorithm 10: EM for any component distribution

Input: number of components m, with components distributions $p(\cdot|\boldsymbol{\theta}_1), \ldots, p(\cdot|\boldsymbol{\theta}_m)$
Initialize $\theta_k^{(0)}$ and $\alpha_k^{(0)}$ for all $k \in 1$ to m, $t = 0$
while not converged **do**
  $p_t[i,k] = \frac{\alpha_k^{(t)} p(\mathbf{x}_i|\boldsymbol{\theta}_k^{(t)})}{\sum_{j=1}^m \alpha_j^{(t)} p(\mathbf{x}_i|\boldsymbol{\theta}_j^{(t)})}$ for all $i \in \{1,2,\ldots,n\}$, $k \in \{1,2,\ldots,m\}$
  Compute $p_t[k] \stackrel{\text{def}}{=} \frac{1}{n}\sum_{i=1}^n p_t[i,k]$
  for $k \in \{1,2,\ldots,m\}$ **do**
    $\alpha_k^{(t+1)} = p_t[k]$
    $\boldsymbol{\theta}_k^{(t+1)} = \text{argmin}_{\boldsymbol{\theta}_k} - \sum_{i=1}^n p_t[i,k] \ln p(\mathbf{x}_i|\boldsymbol{\theta}_k)$
  $t \leftarrow t+1$
return $\alpha_k^t, \boldsymbol{\theta}_k^{(t)}$ for all $k \in \{1,2,\ldots,m\}$

Exercise

- Can we take a mixture over VAE components?
  - Yes! Not sure its useful, but seems fun. Go back to the MM algorithms and see if you can figure out how to do it by
- Is this still easy to evaluate, in terms of negative log-likelihood?

Chapter 15: Missing Data

- Understand how to do imputation using PCA (matrix factorization), including training with missing data and using the model for new data
- Understand how to do imputation using an autoencoder, including training with missing data and using the model for new data
- Understand the difference between the two stage approach (impute then hand to learning algorithm) versus the direct approach (missingness indicator)
- **Will not be tested**
  - Connections to the transductive and semi-supervised settings

Notation check

- What does $\mathbf{x}_{\mathcal{A}_i}$ mean?

Notation check

- What does $\mathbf{x}_{\mathcal{A}_i}$ mean?
- The entries in $\mathbf{x}$ that correspond to the indices in $\mathcal{A}_i$
- We write $\mathbf{x}_{\mathcal{M}_i}$ to refer to the part of the array where values are missing. We use this to talk about directly optimizing for $\mathbf{x}_{\mathcal{M}_i}$

Exercise: PCA (matrix completion)

- In PCA we solved for $\min_{\mathbf{h}_1,\mathbf{h}_2,\ldots,\mathbf{h}_n \in \mathbb{R}^p, \mathbf{D} \in \mathbb{R}^{p \times d}} \sum_{i=1}^{n} \sum_{j=1}^{d} (x_{ij} - \mathbf{h}_i \mathbf{D}_{:j})^2$
- In PCA with missing data, $\min_{\mathbf{h}_1,\mathbf{h}_2,\ldots,\mathbf{h}_n \in \mathbb{R}^p, \mathbf{D} \in \mathbb{R}^{p \times d}} \sum_{i=1}^{n} \sum_{j \in \mathcal{A}_i} (x_{ij} - \mathbf{h}_i \mathbf{D}_{:j})^2$
- Q: Why didn't we just set $\mathbf{x}_{\mathcal{M}_i} = \mathbf{0}$ (set unavailable values to zero) and call PCA? Will we get back the same h's and D as using the above optimization?

Exercise: PCA (matrix completion)

- In PCA we solve for $\min_{\mathbf{h}_1,\mathbf{h}_2,\ldots,\mathbf{h}_n\in\mathbb{R}^p,\mathbf{D}\in\mathbb{R}^{p\times d}} \sum_{i=1}^{n}\sum_{j=1}^{d}(x_{ij}-\mathbf{h}_i\mathbf{D}_{:j})^2$
- In PCA with missing data, $\min_{\mathbf{h}_1,\mathbf{h}_2,\ldots,\mathbf{h}_n\in\mathbb{R}^p,\mathbf{D}\in\mathbb{R}^{p\times d}} \sum_{i=1}^{n}\sum_{j\in\mathscr{A}_i}(x_{ij}-\mathbf{h}_i\mathbf{D}_{:j})^2$
- Q: Why didn't we just set $\mathbf{x}_{\mathscr{M}_i}=\mathbf{0}$ (set unavailable values to zero) and call PCA? Will we get back the same h's and D as using the above optimization?
  - No. But we do if we explicitly minimize over $\mathbf{x}_{\mathscr{M}_i}$

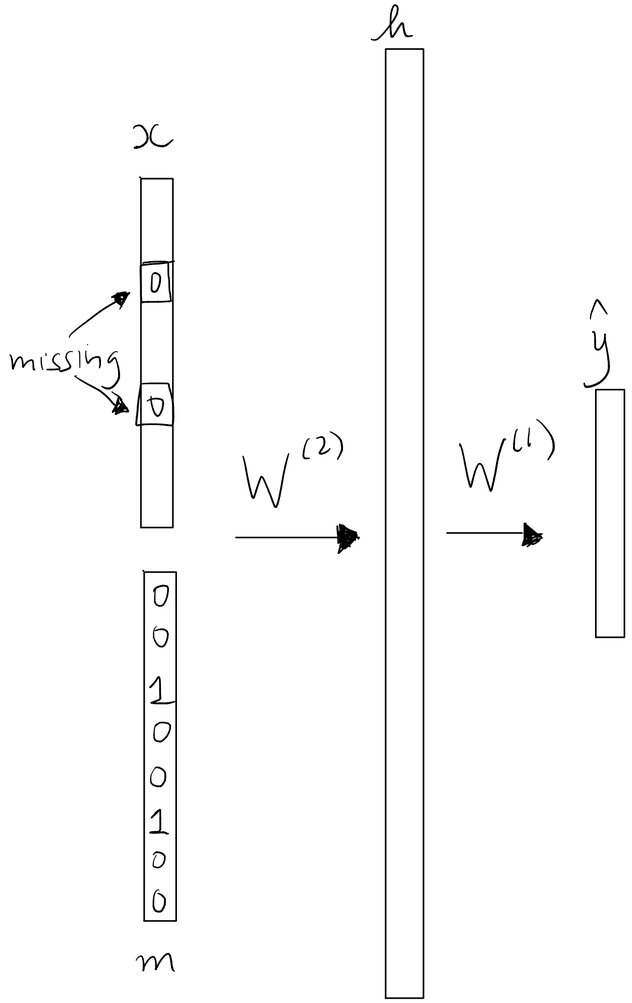
More general loss we use

- In PCA we solve for $\min_{\mathbf{x}_{1,\mathscr{M}_1},\ldots,\mathbf{x}_{n,\mathscr{M}_n}} \min_{\mathbf{h}_1,\mathbf{h}_2,\ldots,\mathbf{h}_n \in \mathbb{R}^p, \mathbf{D} \in \mathbb{R}^{p\times d}} \sum_{i=1}^{n}\sum_{j=1}^{d} (x_{ij} - \mathbf{h}_i \mathbf{D}_{:j})^2$
- For autoencoder, $\min_{\mathbf{x}_{1,\mathscr{M}_1},\ldots,\mathbf{x}_{n,\mathscr{M}_n}} \min_{\mathbf{W}} \sum_{i=1}^{n}\sum_{j=1}^{d} (x_{ij} - f_{\mathbf{W}}(\mathbf{x}_i))^2$
- We need this more general purpose loss for the autoencoder, because we cannot use the following objective. **Why**?

  $\min_{\mathbf{W}} \sum_{i=1}^{n}\sum_{j\in\mathscr{A}_i} (x_{ij} - f_{\mathbf{W}}(\mathbf{x}_i))^2$

Exercise

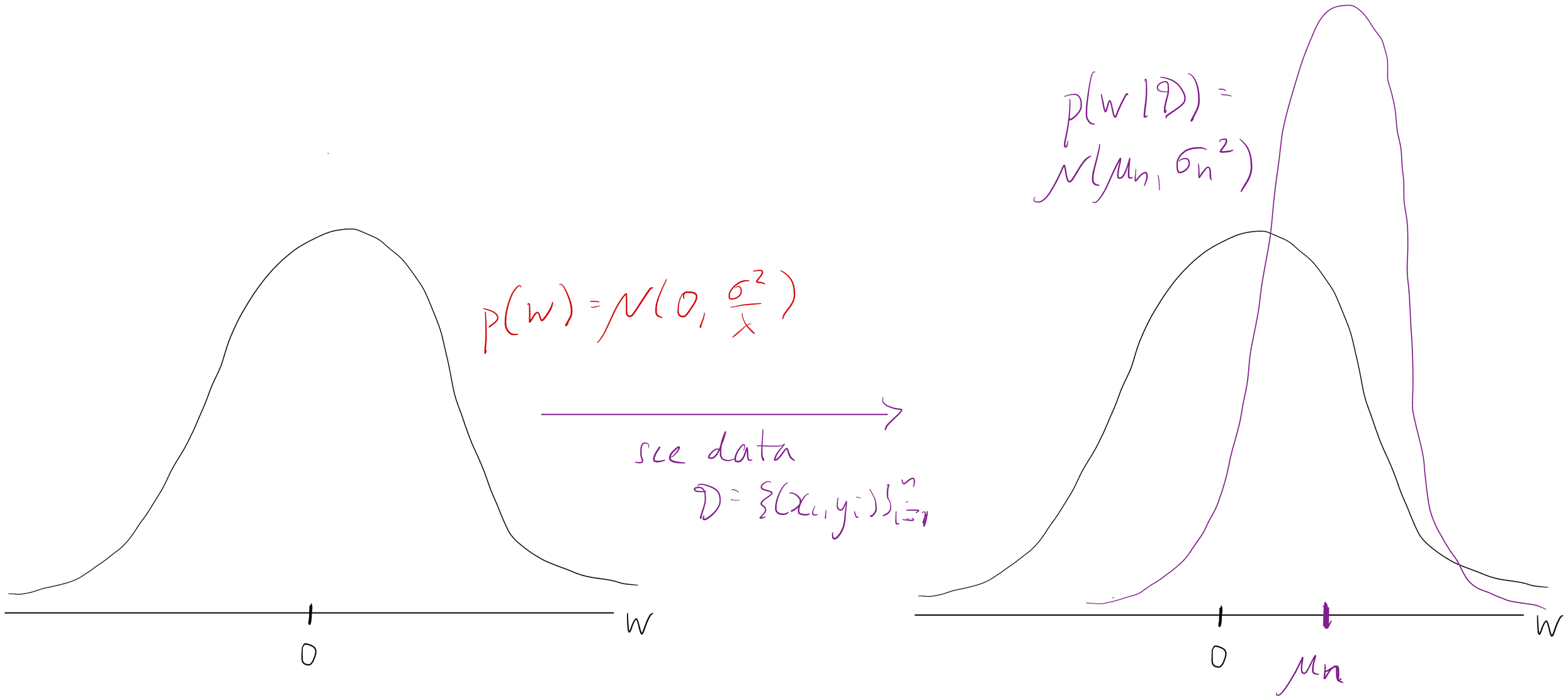
- Our goal in direct prediction was to learn an NN that conditions on $(\mathbf{x}_{\mathscr{A}}, \mathscr{M})$
- What if we knew that we would only ever see feature 1 or feature 2 missing. We decide to train three NNs: one using only features 2 to d, one using only features 1, 3 to d and one using all features.
- Q: In deployment, how do you use these three models?
- Q: How might you train these?
- Q: Is this also learning a model that conditions on $(\mathbf{x}_{\mathscr{A}}, \mathscr{M})$?



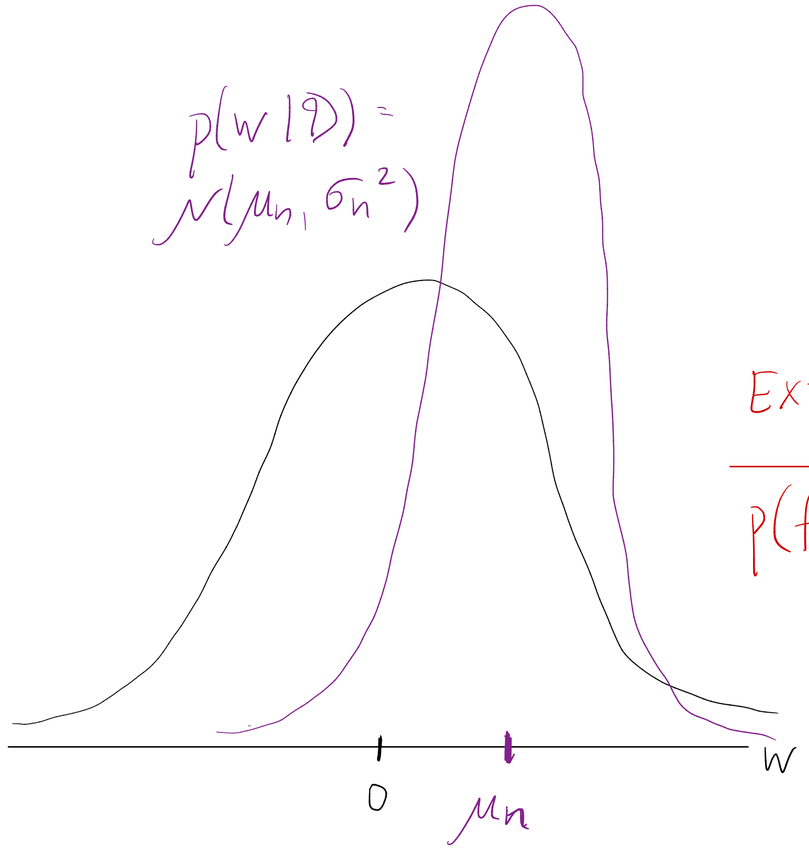
Chapter 15: Uncertainty estimation

- Understand that we might want to know distribution over plausible values of $\mathbf{w}$, given the evidence (data)
- Understand that this allows us to also obtain a distribution over our predictions, and so construct credible intervals $[f_{\mathbf{w}}(\mathbf{x}) - \epsilon, f_{\mathbf{w}}(\mathbf{x}) + \epsilon]$
- Understand why the posterior and credible interval shrink with growing n
- **Will not test you on**
  - Memorizing the formulas for Bayesian linear regression
  - The Normal-inverse gamma distribution

Shrinking posterior

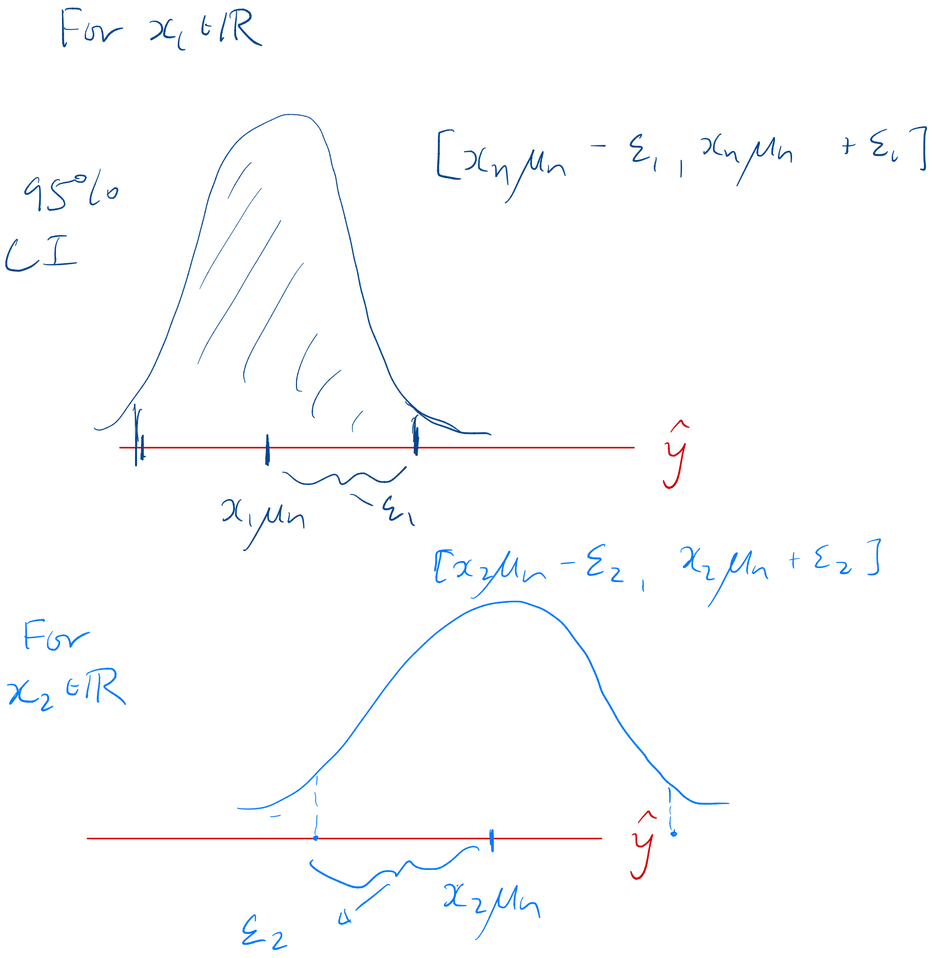


Credible Interval for Predictions



Extract

$p(f_w(x)|D)$

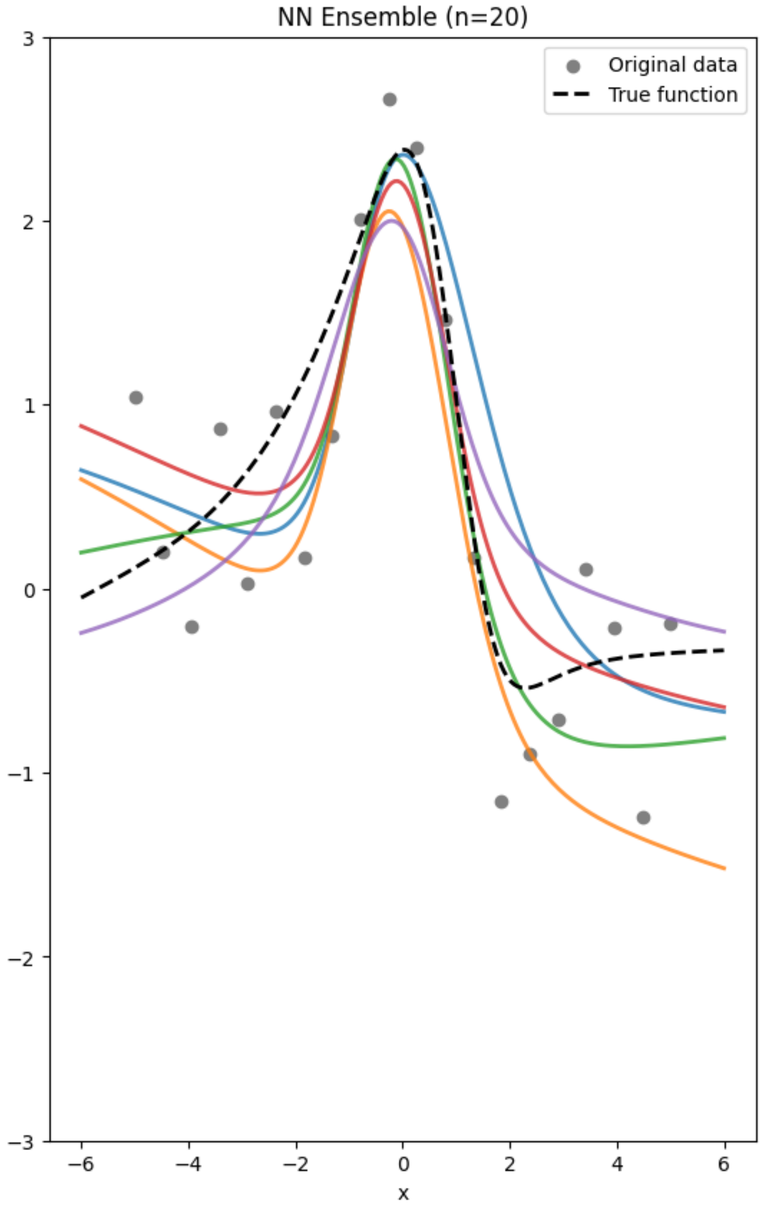


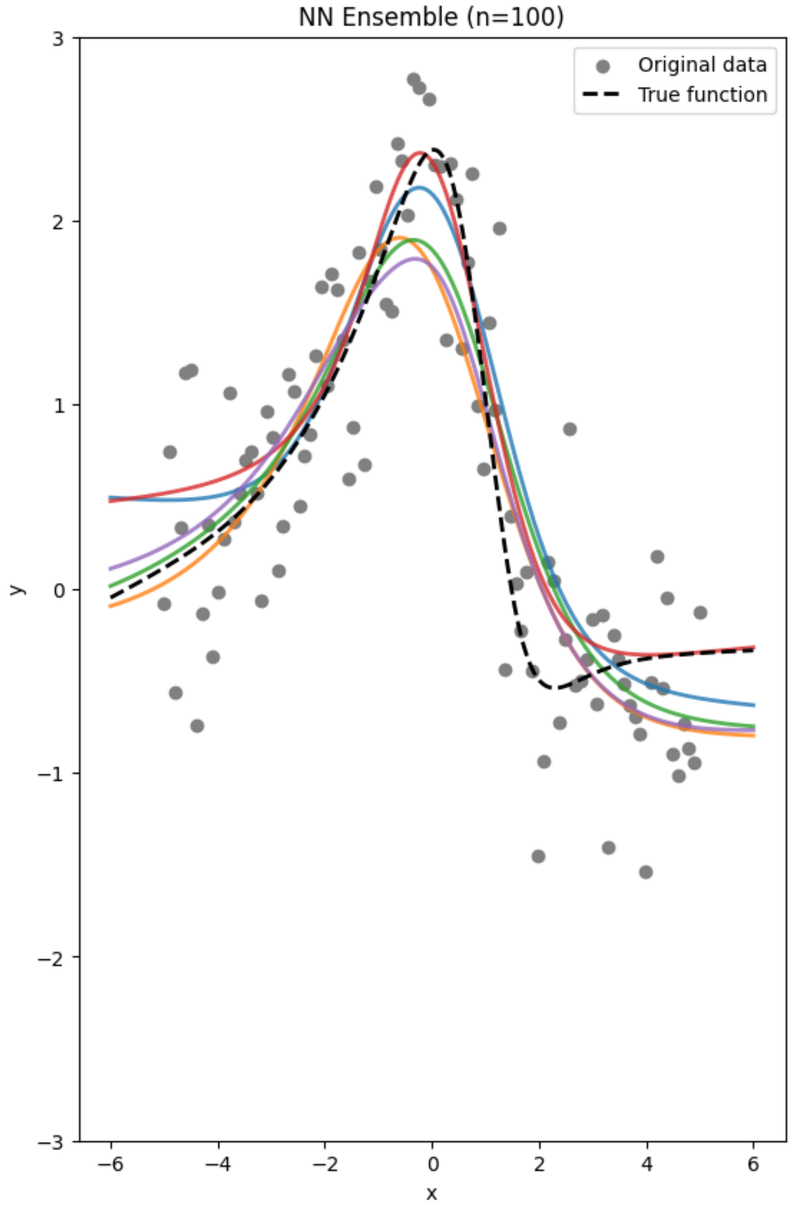
Chapter 16: Uncertainty estimation

- Understand that we can use fixed representations + Bayesian linear regression to get nonlinear regressors + credible intervals
- Understand that we can use bootstrap resampling to estimate uncertainty for neural networks
  - Understand that we sample m datasets with replacement from all the training data, and that we train an NN $f_{\mathbf{W}_k}$ from scratch on each dataset k
  - We use this ensemble of NNs to get a set of predictions to compute intervals for our predictions, $\hat{y}_1 = f_{\mathbf{W}_1}(\mathbf{x}), \ldots, \hat{y}_m = f_{\mathbf{W}_m}(\mathbf{x})$
- **Will not test:** how to compute percentile CIs

Discussion

- Looking at the ensembles learned, what can you say? Can you hypothesize what subset of points were used to train the yellow line?
- Why are the lines so much more similar for n = 100, even though the data is just as variable?
- If we had n = 10,000, what might you expect to see for our ensemble of m = 5?





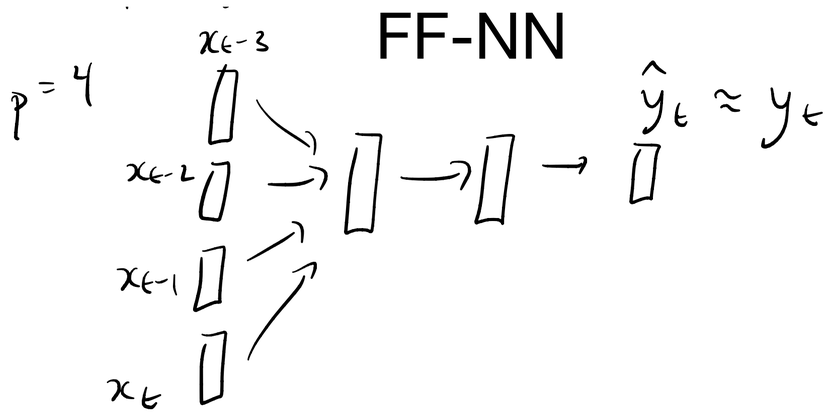
Chapter 17: Learning on temporal data

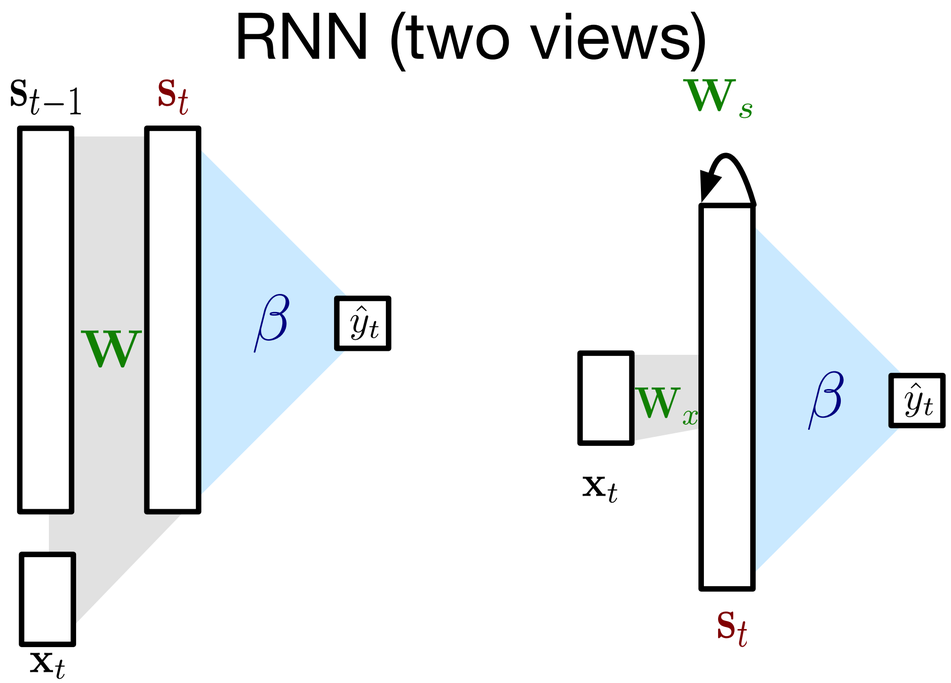
- Understand that data is of the form $\{(\mathbf{x}_1, \mathbf{y}_1), (\mathbf{x}_2, \mathbf{y}_2), \ldots (\mathbf{x}_t, \mathbf{y}_t)\}$ where now index indicates time: i-1 happened before i, which happened before i+1, etc.
- Understand that these temporal relationships allow us to mitigate partial observability by conditioning on the history rather than just the immediate observation: predicting $\mathbf{y}_t$ using $\mathbf{x}_1, \ldots, \mathbf{x}_{t-1}, \mathbf{x}_t$ rather than just $\mathbf{x}_t$
- Understand our two key strategies:
  - conditioning explicitly on the last p points, inputting them into our function (NN)
  - using recurrence to incrementally summarize and construct state
- Understand transformers use first approach, but allow for large p by construction

Exercise

- Consider the three NN choices we considered
  - **Option 1**: stack the last p observations $\mathbf{x}_{t-p}, \ldots, \mathbf{x}_t$ and input to a standard feedfoward NN (e.g., multiple ReLU layers)
  - **Option 2**: use a recurrent neural network (RNN) (e.g., simple single hidden recurrent layer with ReLU, or more advanced RNNs like GRU, LSTM)
  - **Option 3**: the last p observations $\mathbf{x}_{t-p}, \ldots, \mathbf{x}_t$ into a transformer (a particular NN architecture)

The three architectures





Transformer subblock

before linearly combining and sending to layernorm+ReLU

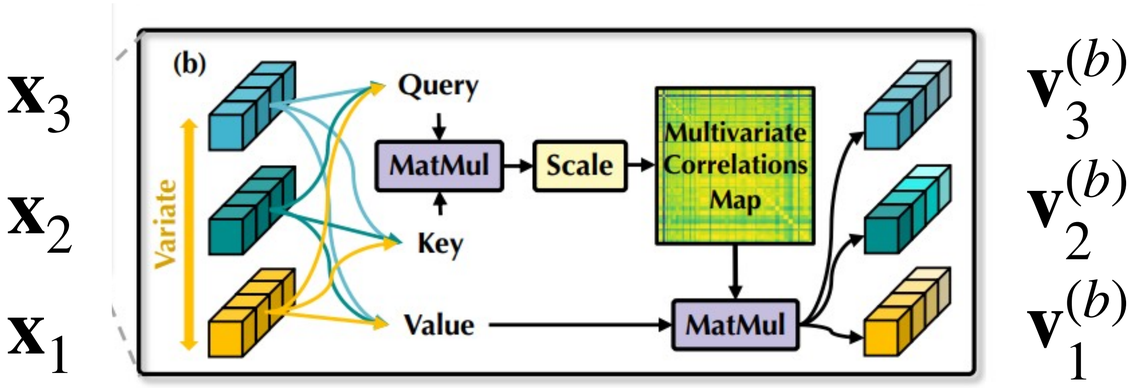


*image from
https://www.analyticsvidhya.com/blog/2024/05/a-comprehensive-guide-on-i-transformer/

Exercise

- Consider the weights for our three NN choices we considered
  - Option 1: stack the last p observations $\mathbf{x}_{t-p}, \ldots, \mathbf{x}_t$ and input to a standard feedfoward NN (e.g., multiple ReLU layers)
  - Option 2: use a recurrent neural network (RNN) (e.g., simple single hidden recurrent layer with ReLU, or more advanced RNNs like GRU, LSTM)
  - Option 3: the last p observations $\mathbf{x}_{t-p}, \ldots, \mathbf{x}_t$ into a transformer (a particular NN architecture)
- Q: Does the number of parameters grow with increasing p for the FFNN, the RNN, and/or the Transformer?
  How about with increasing observation dimension d?

Exercise

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  - Option 1: stack the last p observations $\mathbf{x}_{t-p}, \ldots, \mathbf{x}_t$ and input to a standard feedfoward NN (e.g., multiple ReLU layers)
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  - Option 3: the last p observations $\mathbf{x}_{t-p}, \ldots, \mathbf{x}_t$ into a transformer (a particular NN architecture)
- Q: Does the number of parameters grow with increasing p for the FFNN, the RNN, and/or the Transformer? How about with increasing observation dimension d?
- **Ans**: #parameters grows with increasing d for all three, #parameters grows with increasing p for FNN, but not for RNN or Transformer

Exercise

- All of our approaches created a new representation that summarizes the history
  - Option 1: input last p observations $\mathbf{x}_{t-p}, \ldots, \mathbf{x}_t$ to feedfoward NN produces final hidden layer $\mathbf{h}^{(1)}$
  - Option 2: Recurrence is a state update function, that provides current compact summary of sequence:
  - Option 3: input last p observations $\mathbf{x}_{t-p}, \ldots, \mathbf{x}_t$ to Tranformer produces $\mathbf{z}_{t-p}, \ldots, \mathbf{z}_t$ where we used $\mathbf{z}_t$ as our new representation
- Q: How do we use this new representation? Do we always use it to predict $\mathbf{x}_{t+1}$?

Exercise

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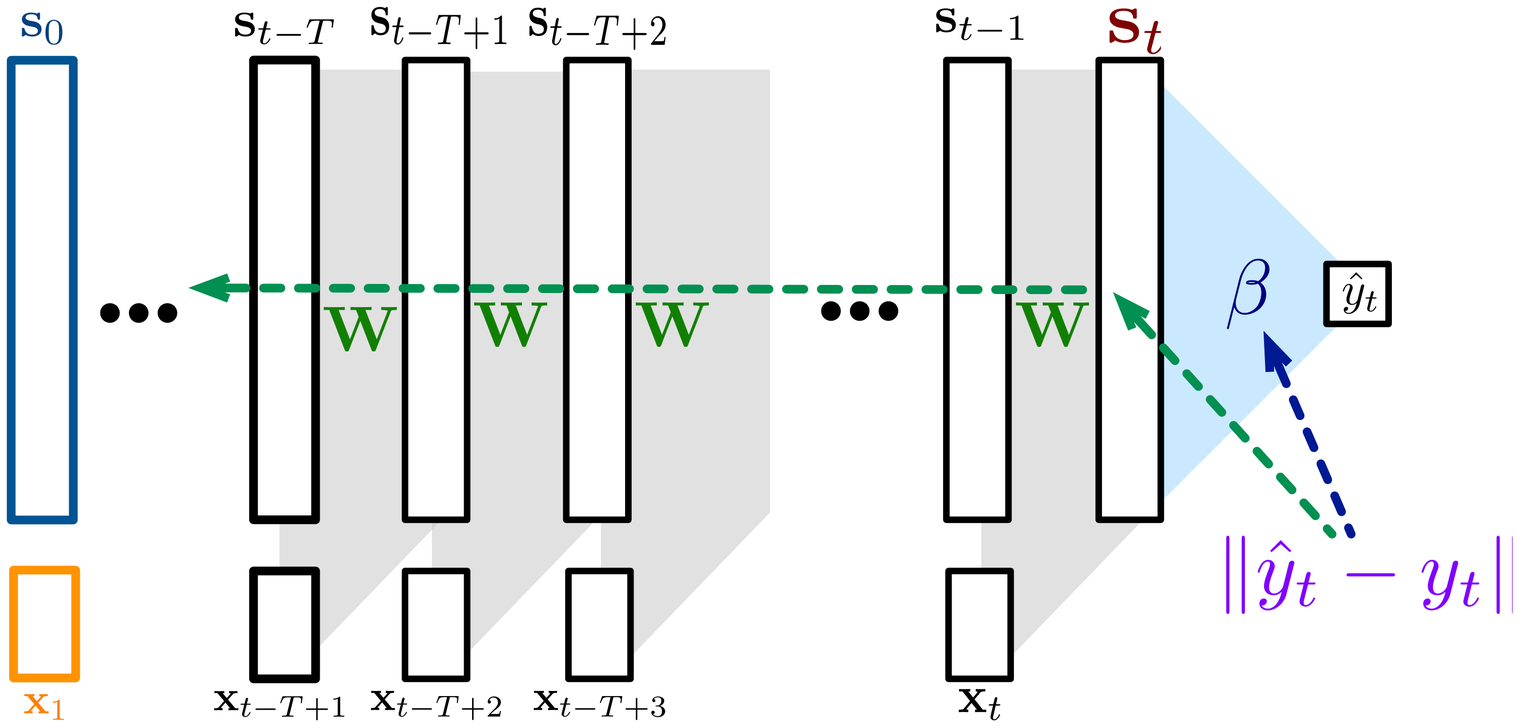
- Q: How do we use this new representation? Do we always use it to predict $\mathbf{x}_{t+1}$?
  - No. Like any NN, we can use it to predict any target we want. Can predict $\mathbf{x}_{t+10}$ or could predict something not in the time series, such as a classification target (e.g., does the image in a sequence contain a cat or not)

Chapter 17: Learning on temporal data (cont.)

- Understand all three approaches are trained using gradient descent (backprop), but that for an RNN this involves unrolling the recurrence (computing the gradients back in time, called backprop through time)
- Understand a predicted sequence can be generated autoregressively: predict $\hat{\mathbf{x}}_{t+1}$, then use your own prediction to predict $\hat{\mathbf{x}}_{t+2}$, etc.
- **Will not be directly tested**
  - The Transformer architecture and any specific RNN architectures
  - Do not need to know nuances around training RNNs with backprop, including how to pick truncation, how to use mini-batches, etc.

Discussion: BPTT for an RNN vs backprop for a transformer

- Why don’t we say a transformer is using BPTT? It is also looking at the sequence back in time?
- Why might an RNN with BPTT be more prone to vanishing or exploding gradients?
- For a feedforward NN, do we use BPTT or standard backprop?



Chapter 18: Gen error beyond iid

- Entire chapter will not be tested