MS&E 228: Modern Non-Linear Prediction

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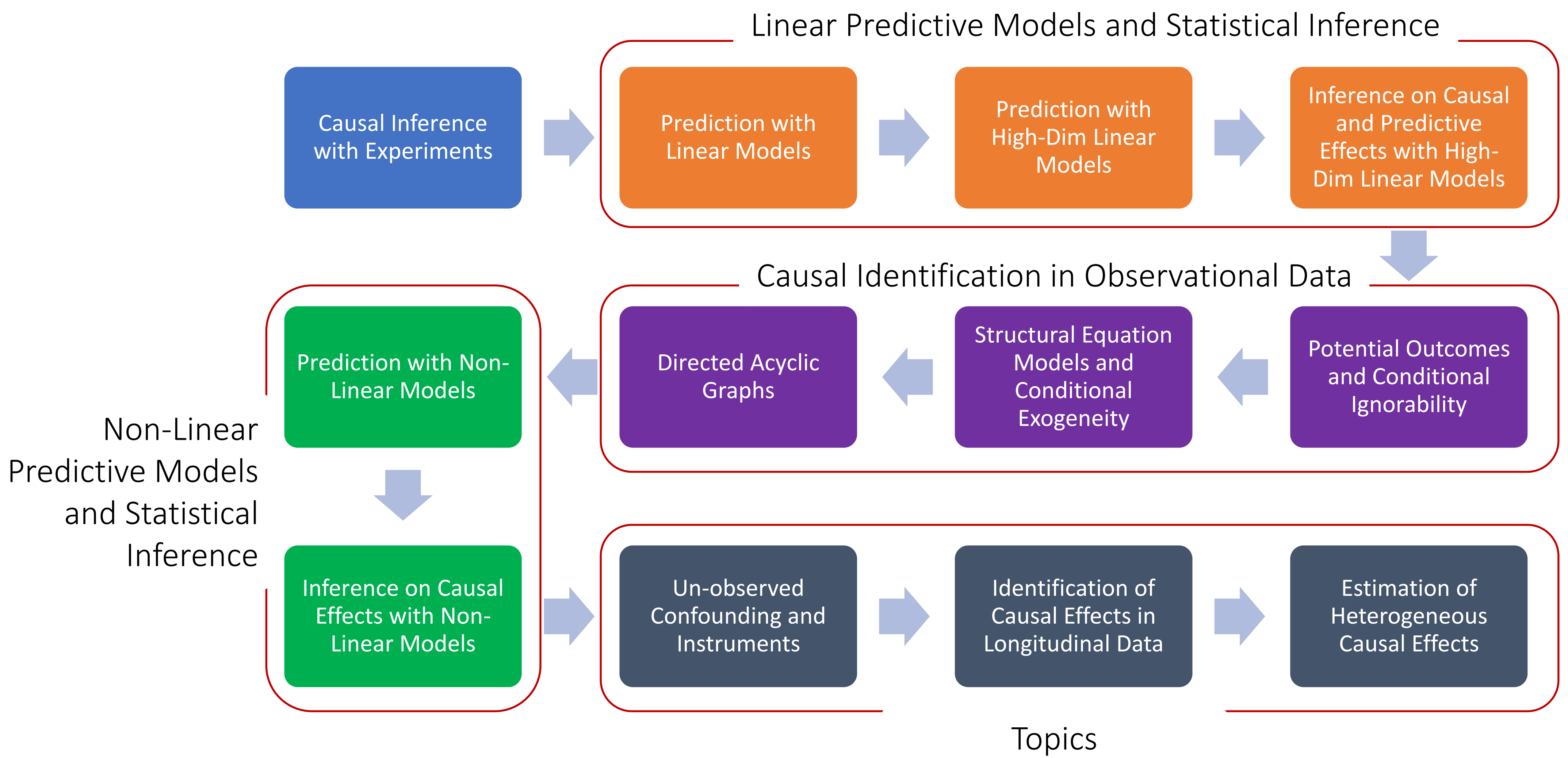
Linear Predictive Models and Statistical Inference
Causal Inference with Experiments
Prediction with Linear Models
Prediction with High-Dim Linear Models
Inference on Causal and Predictive Effects with High-Dim Linear Models
Causal Identification in Observational Data
Potential Outcomes and Conditional Ignorability
Structural Equation Models and Conditional Exogeneity
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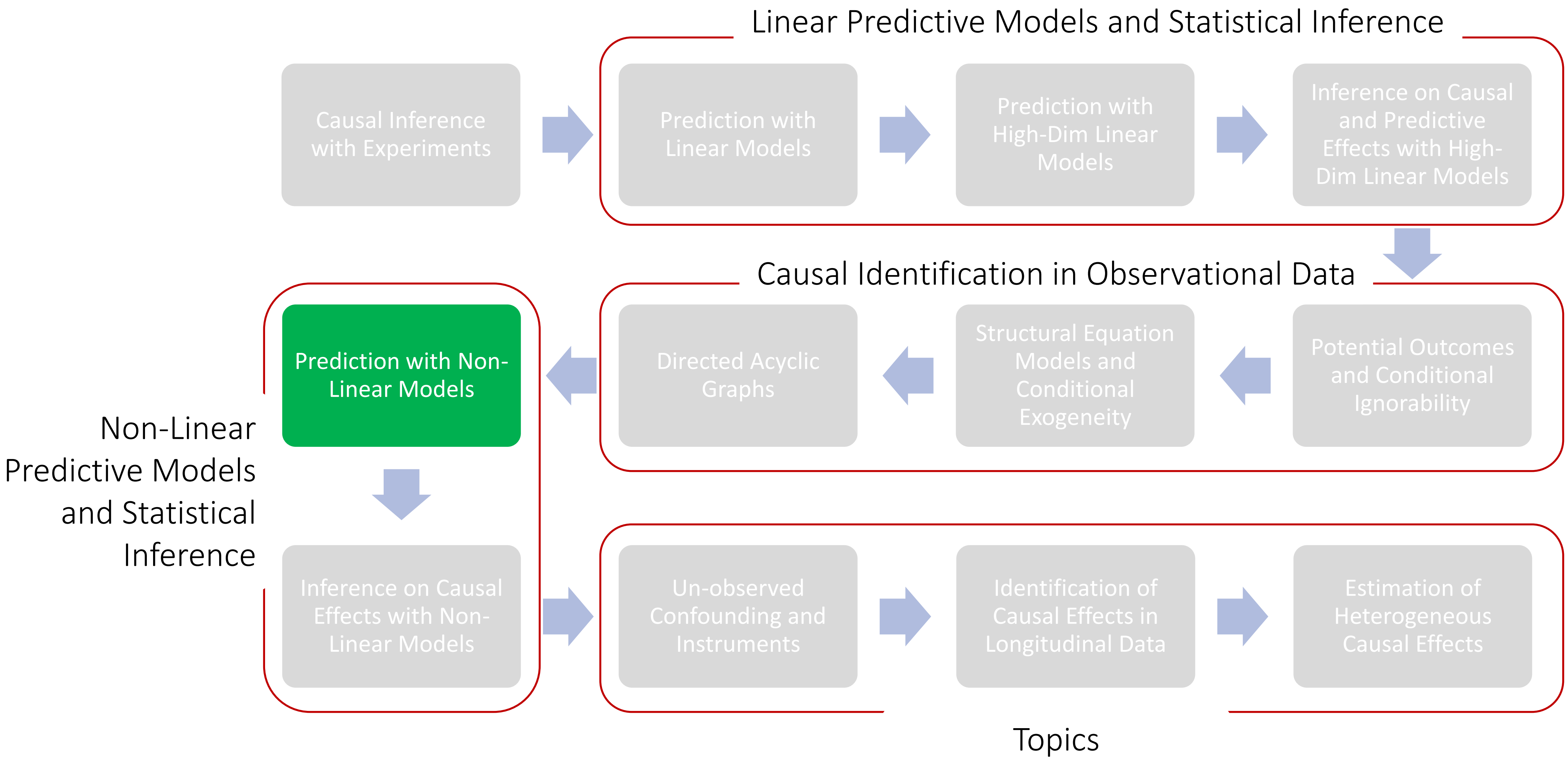
Un-observed Confounding and Instruments
Identification of Causal Effects in Longitudinal Data
Estimation of Heterogeneous Causal Effects
Topics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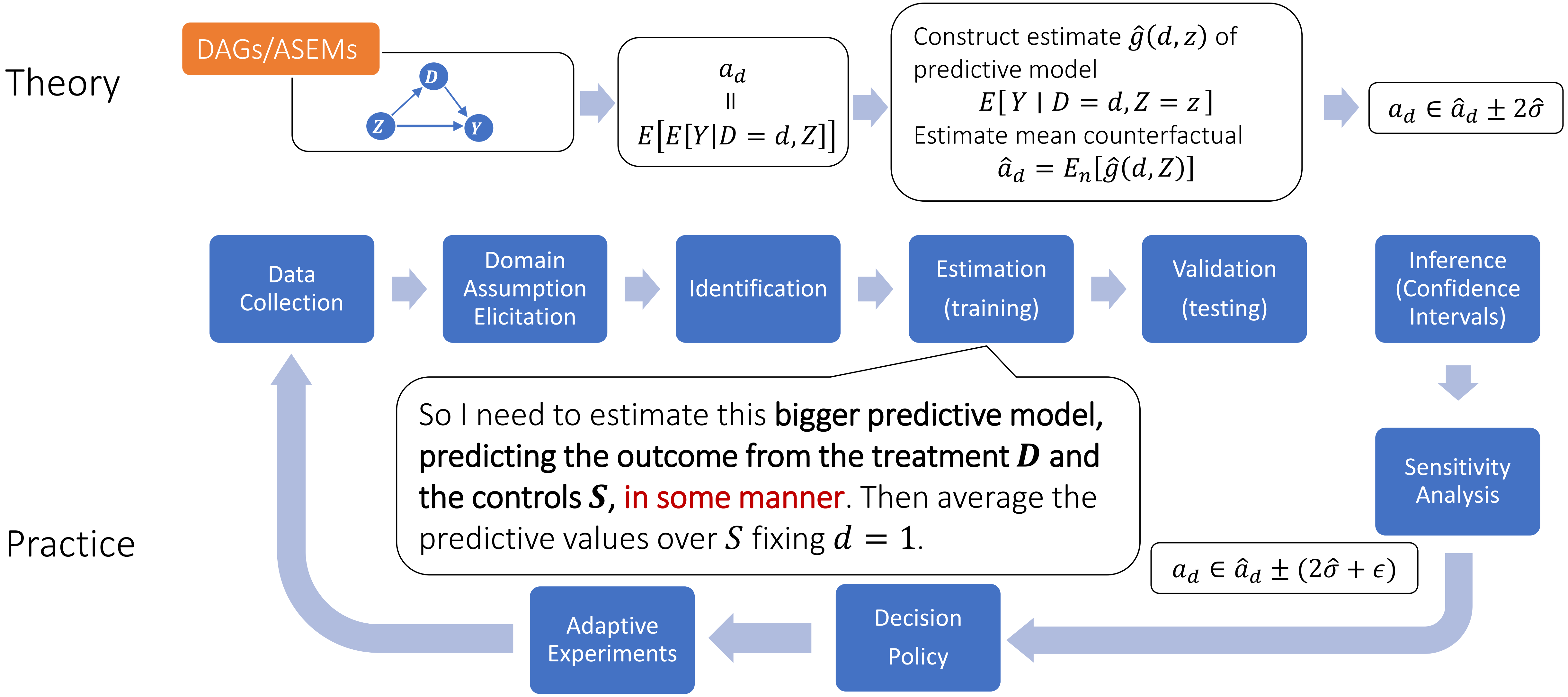
Recap of Last Lecture

Causal Inference Pipeline



Problem Statement

- Given n samples $(Z_1, Y_1), \dots, (Z_n, Y_n)$ drawn iid from a distribution D
- Want an estimate $\hat{g}$ that approximates the Best Prediction

$$g := \operatorname*{argmin}_{\tilde{g}} E\left[\left(Y - \tilde{g}(Z)\right)^2\right]$$

- Best Prediction rule is Conditional Expectation Function (CEF)

$$g(Z) = E[Y|Z]$$

- We want our estimate $\tilde{g}$ to be close to g in RMSE

$$\|\hat{g} - g\| = \sqrt{E_Z\left(\hat{g}(S) - g(Z)\right)^2} \to 0, \qquad \text{as } n \to \infty$$

The Curse of Dimensionality

- What if we make no real assumption on $g(Z) \coloneqq E[Y|Z]$
- Suppose we only assume g is a smooth function
- Formal form of smoothness: g is β-smooth if it has uniformly bounded and continuous β-high order derivatives

- Classic non-parametric statistics [Stone'82]: provably best you can do

$$||g - \hat{g}|| \approx n^{-\frac{\beta}{2\beta+p}}$$

Bypassing the Curse of Dimensionality

- Lasso scaled to $p \gg n$ by adapting to notions of “effective dimension” (e.g. s/n, with s is number of relevant variables)
- We need methods with similar behavior for non-linear models

- Many modern machine learning techniques achieve exactly that
- Their error scales with appropriate notions of “effective dimension”

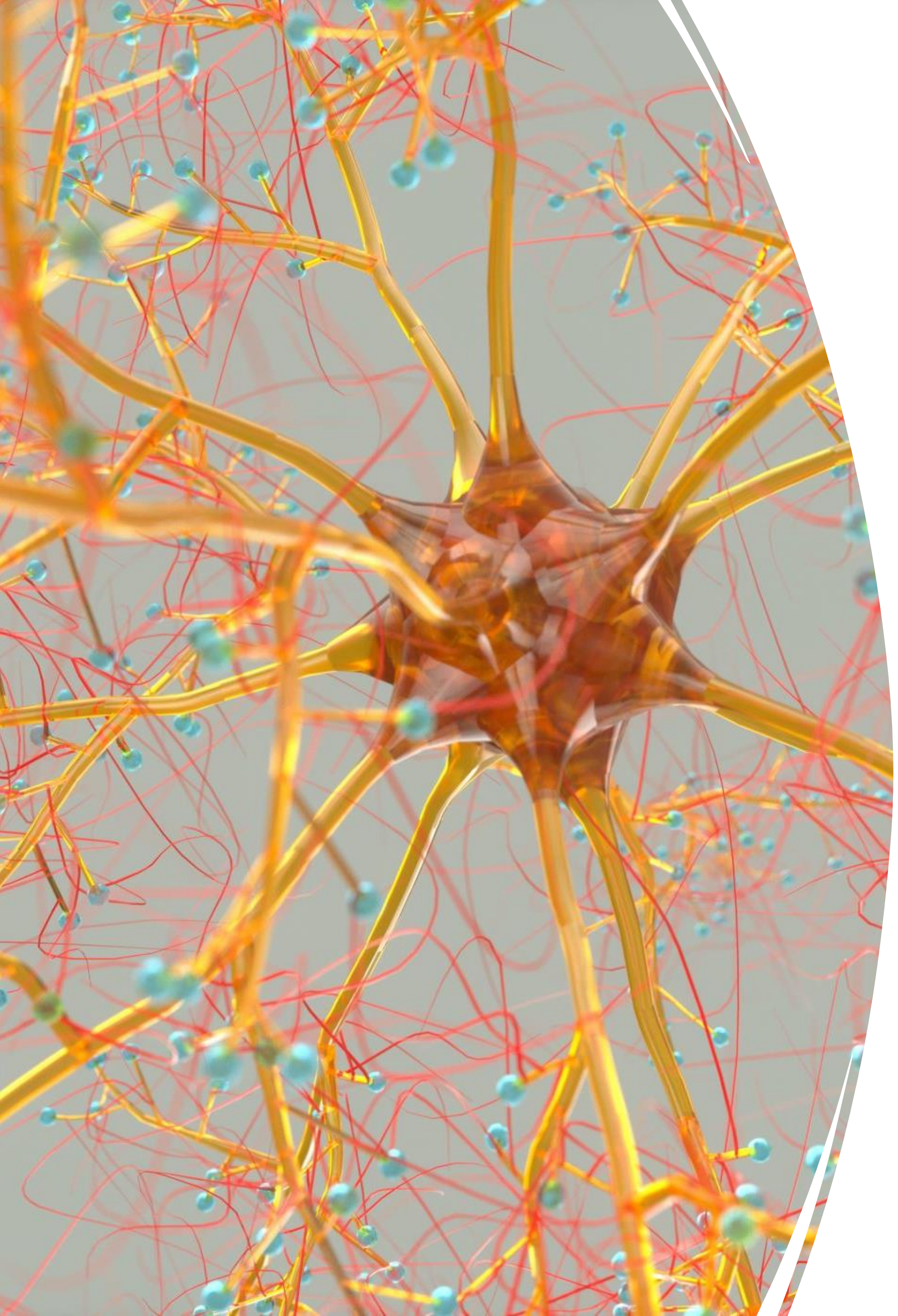
- Last time: Regression Trees, Random Forests, Gradient Boosted Forests

Goals for Today

- Neural Networks
- Some theoretical guarantees and justification (similar to lasso)
- How to combine models (stacking)
- How to automate the process (automl)

- NNets for feature engineering

Modern Non-Linear Predictive Models: Neural Networks



(Shallow) Neural Networks

- We approximate the CEF with data-driven engineered features
$$g(z) \coloneqq \beta' \phi(z; a)$$
- Typical choice of ϕ is:
$$\phi(z; a) = \sigma(a'z)$$
- With σ some non-linear function

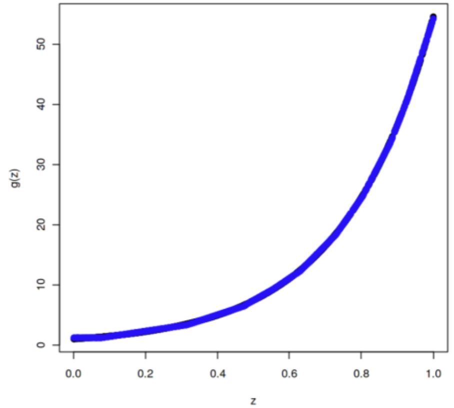
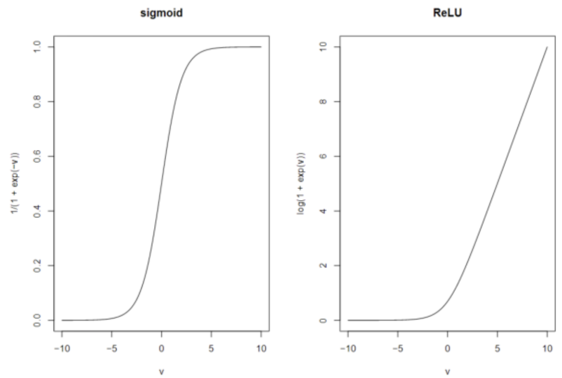


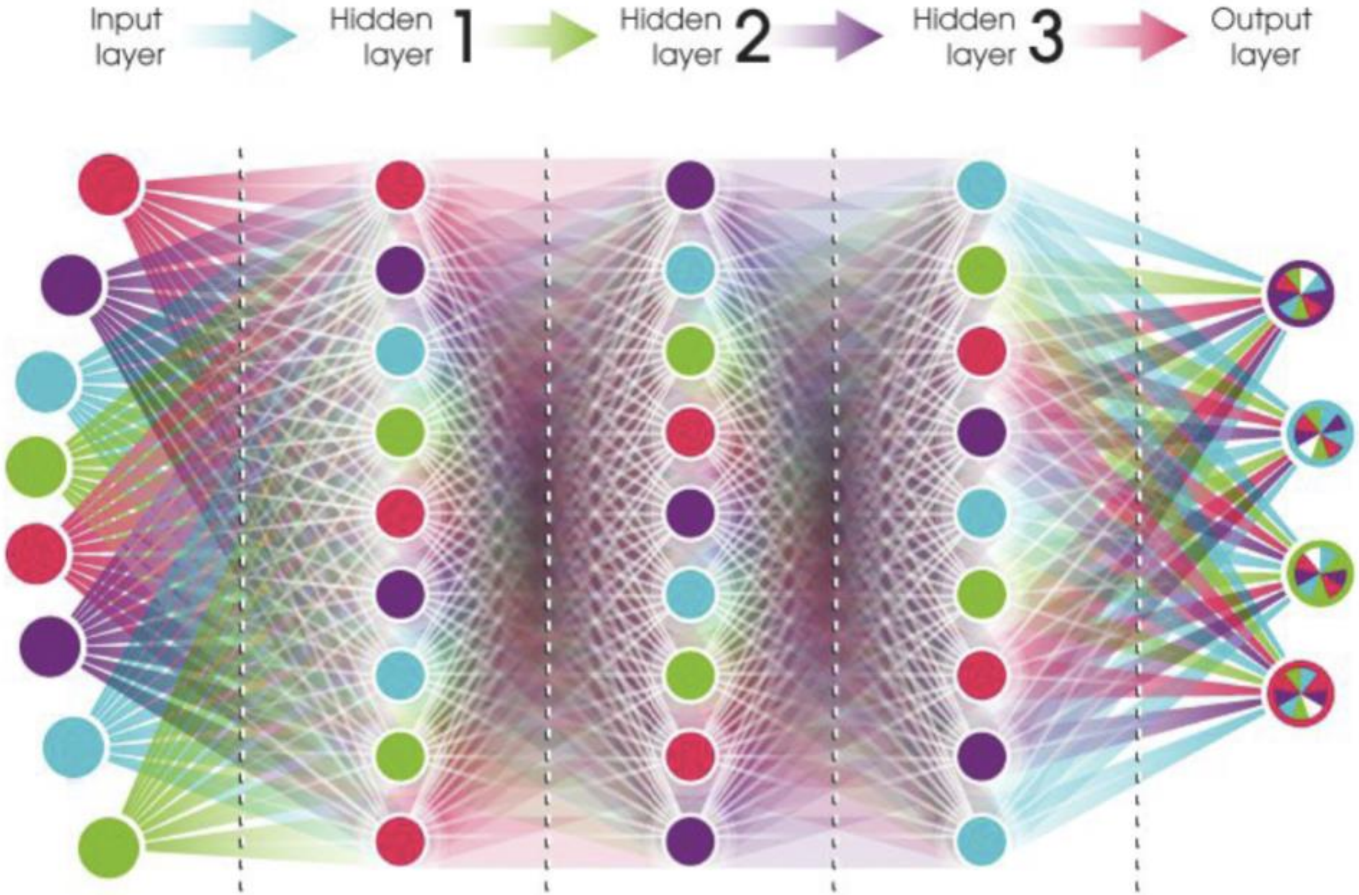
Figure 2.12: Approximation of $g(Z) = \exp(4Z)$ by a Neural Network



(Shallow) Neural Network Objective

- Parameters chosen by minimizing penalized empirical square loss
$$\min_{\alpha,\beta} E_n\left[\left(Y \ - \beta' \phi(Z;\alpha)\right)^2\right] + \lambda \, \mathrm{pen}(a, \beta)$$
- Penalty is either ℓ_1 norm (sparsity inducing) or ℓ_2 norm (inducing small weights); λ is referred as *weight decay* in the case of ℓ_2
- Loss is typically minimized via *Stochastic Gradient Descent* (SGD)
$$(\alpha, \beta) \leftarrow (\alpha, \beta) - \eta \partial_{\alpha,\beta} \mathrm{Loss}(\mathrm{B}; \alpha, \beta)$$
- $\mathrm{Loss}(\mathrm{B}; \alpha, \beta)$ is empirical loss calculated on a sub-sample B (*batch*)
$$\frac{1}{|B|} \sum_{i \in B} \left(Y_i \ - \beta' \phi(Z_i; \alpha)\right)^2 + \lambda \, \mathrm{pen}(a, \beta)$$
- Every pass over all the data is referred to as an *epoch*

DEEP NEURAL NETWORK



neuralnetworksanddeeplearning.com - Michael Nielsen, Yoshua Bengio, Ian Goodfellow, and Aaron Courville, 2016.

Forms of Regularization

- *Stochasticity* and iterative nature of SGD is by itself a regularization method (implicit regularization)
- *Penalties* are explicit form of regularization
- *Drop-out.* At each training step, shutdown some of the neurons. Implicitly regularizes by having multiple neurons learn important concepts, acting as substitutes
- *Early stopping.* Measure out of sample performance after a few iterations of SGD and stop if it stops improving

Let’s check it out!

Some Theory

Structured Sparsity and Smoothness. Assume g is a composition

$$g = f_M \circ \cdots \circ f_0$$

Where i-th function $f_i: \mathbb{R}^{p_i} \to \mathbb{R}^{p_{i+1}}$ has its p_{i+1}components β_i-smooth (*smoothness*) and depends only $t_i \ll p_i$ input variables (*sparsity*); these t_i variables can be different for each component

Effective dimension is $s \coloneqq \max_i n^{\frac{t_i}{2\beta_i + t_i}}$

Theorem[Schmidt-Hieber'20]. If depth$\sim \log(n)$ and width $\geq s \log(n)$, and several other regularity conditions, then error of an appropriately trained neural network is at most $\approx \sqrt{\frac{s}{n}} \mathbf{polylog}(n)$

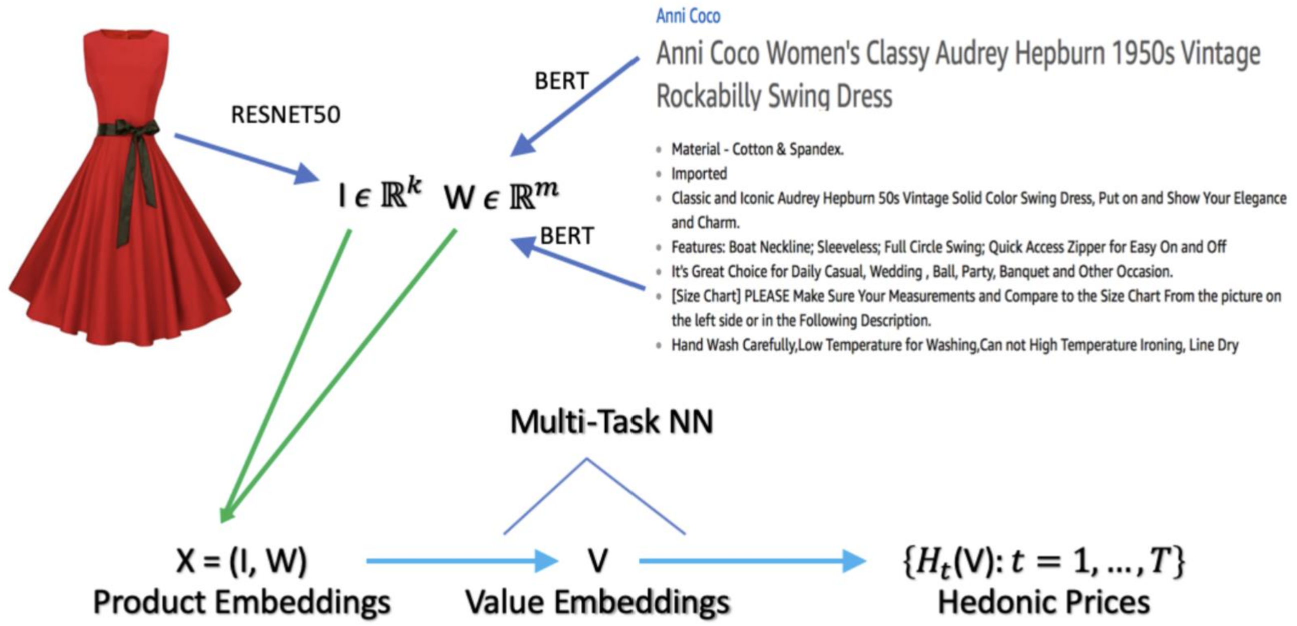
A Reminder: Fancy isn't always better

Predictive performance for predicting wages

	MSE	S.E.	R^2
Least Squares (basic)	0.229	0.016	0.282
Least Squares (flexible)	0.243	0.016	0.238
Lasso	0.234	0.015	0.267
Post-Lasso	0.233	0.015	0.271
Lasso (flexible)	0.235	0.015	0.265
Post-Lasso (flexible)	0.236	0.016	0.261
Cross-Validated Lasso	0.229	0.015	0.282
Cross-Validated Ridge	0.234	0.015	0.267
Cross-Validated Elastic Net	0.230	0.015	0.280
Cross-Validated Lasso (flexible)	0.232	0.015	0.275
Cross-Validated Ridge (flexible)	0.233	0.015	0.271
Cross-Validated Elastic Net (flexible)	0.231	0.015	0.276
Random Forest	0.233	0.015	0.270
Boosted Trees	0.230	0.015	0.279
Pruned Tree	0.248	0.016	0.224
Neural Net	0.276	0.012	0.148

But many times it is crucial

Predicting prices from product characteristics at Amazon



Bajari et al. 2021, *Hedonic prices and quality adjusted price indices powered by AI*.

Which method should I use?

Stacking and Ensembling

Use all and combine: Stacking

- If you have many models $\hat{g}_1, \ldots, \hat{g}_K$ we can combine based on out-of-sample performance

$$\begin{aligned}
\text{Best} - \text{Loss} &= \min_k E\left[\left(Y - \hat{g}_k(Z)\right)^2\right] \\
&= \min_{w \geq 0: \sum_k w_k = 1} \sum_k w_k E\left[\left(Y - \hat{g}_k(Z)\right)^2\right] \\
&\geq \min_{w \geq 0: \sum_k w_k = 1} E\left[\left(Y - \sum_k w_k \, \hat{g}_k(Z)\right)^2\right] = \text{Loss of Best Ensemble}
\end{aligned}$$

Stacking

- Train an OLS on the out-of-sample data predicting Y with features $g_1(Z), \ldots, g_K(Z)$ to learn weights w; return ensemble prediction

$$\hat{g}(Z) \coloneqq \sum_{k=1}^{K} w_k \hat{g}_k(Z)$$

- If models are too many, we can train Lasso on out-of-sample to learn weights, to avoid overfitting!

Let's check it out!

How do I choose all these hyperparameters?

Use Auto-ML frameworks!

- Automatic and clever search over the hyperparameter space
- Very few lines of code
- Typically much better performance than handpicking yourself
- Unless a lot of domain knowledge of what types of functions are better approximators

- Many user-friendly tools: H2O-AutoML, Auto-Gluon, Azure-AutoML, FLAML, Auto-Sklearn, HyperOpt-Sklearn

Feature Engineering with Pre-Trained Neural Networks

PCA, Large Language Models, Large Vision Models

Auto-Encoders

Reducing Dimensionality via Latent Embeddings

- Suppose we have a high dimensional set of variables $W \in \mathbb{R}^p$

- One way to address the curse of dimensionality: find an equally good low dimensional representation of W

- Find small set of features $X \in \mathbb{R}^K$ that "capture all information in W"

Reconstruction Error Objective

- We should be able to predict (reconstruct) W very accurately from X

- For every original feature W_j we can predict it well from features X

$$\min_{a_j} E_n\left[\left(W_j - a_j'X\right)^2\right] \ll \epsilon$$

- Overall, the following *reconstruction error* should be small

$$\min_{a_1,\ldots,a_p} \sum_{j=1}^{p} E_n\left[\left(W_j - a_j'X\right)^2\right] = \min_{A} E_n\left[\|W - A'X\|_2^2\right]$$

Principal Components

- Popular approach: find $X_1, \ldots, X_K$ that are un-correlated
- Each feature captures an independent (orthogonal) dimension of variation of the original variables W

- Find K orthogonal projections of the original variables

$$X_k = c_k' W$$

$$c_k' c_j = 0 \text{ and } c_k' c_k = 1 \text{ and } E\left[X_k X_j\right] = 0 \ (k \neq j)$$

- The best such set of projections $c_1, \ldots, c_k$ such that the "reconstruction error" is minimized is the principal components! (top eigenvectors of cov. matrix $E_n[WW']$)

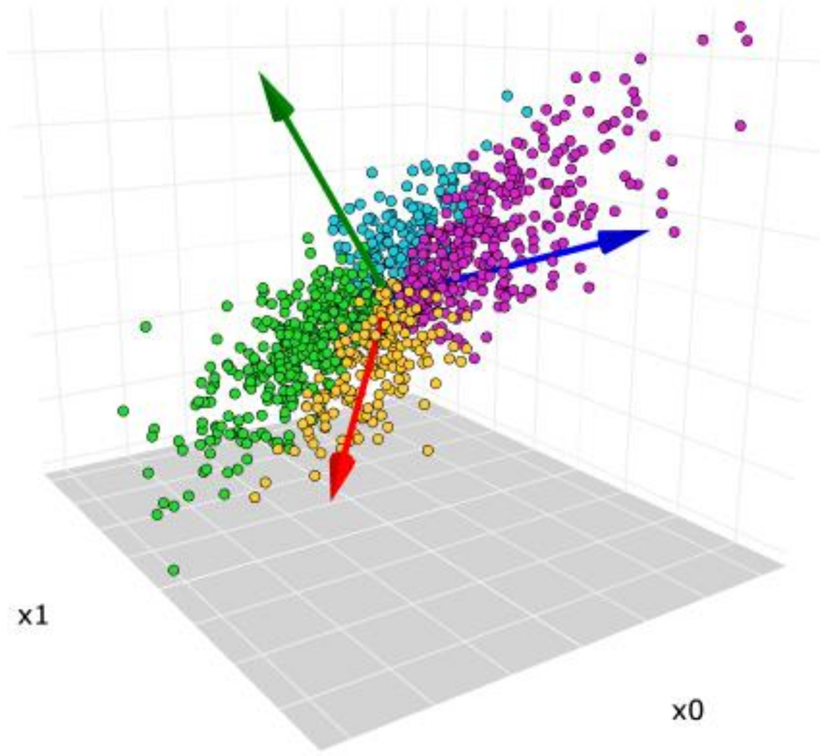


Image Source: https://towardsdatascience.com/principal-component-analysis-pca-explained-visually-with-zero-math-1cbf392b9e7d

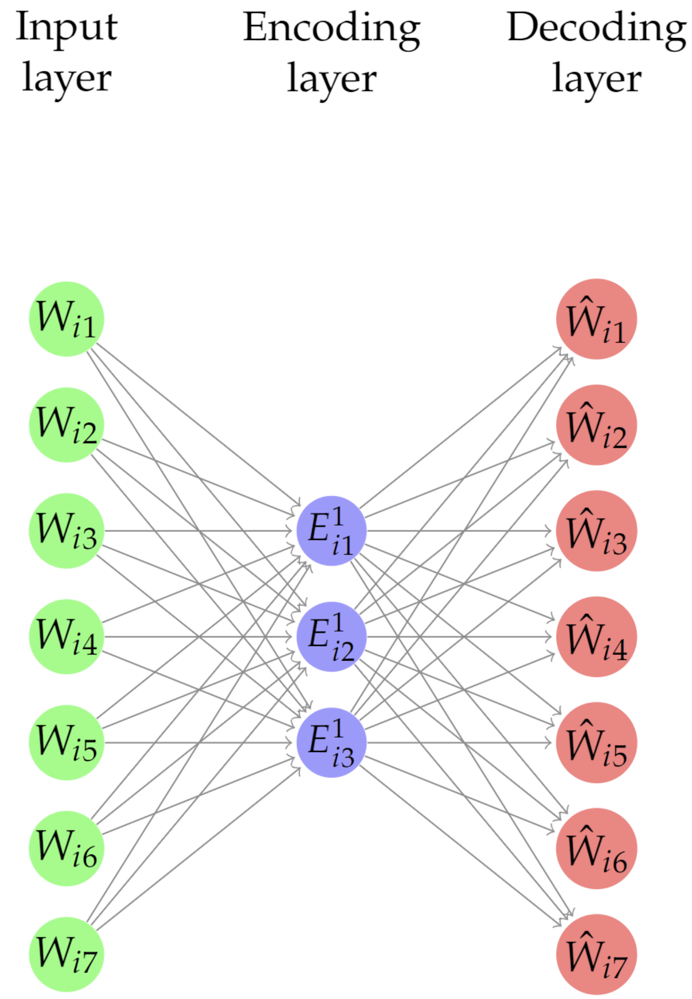
Principal Components as Encoders-Decoders

- Principal components encode the original data with a linear transform

$$W \to C_K' W \coloneqq E \to A' E =: \widehat{W}$$

- "Encoding" process takes a high-dimensional set of features and "encodes" them or "embeds" them in a low dimensional space
- "Decoding" process takes an "encoding" or "embedding" in this low dimensional space and reconstructs the original set of features in the high-dimensional space

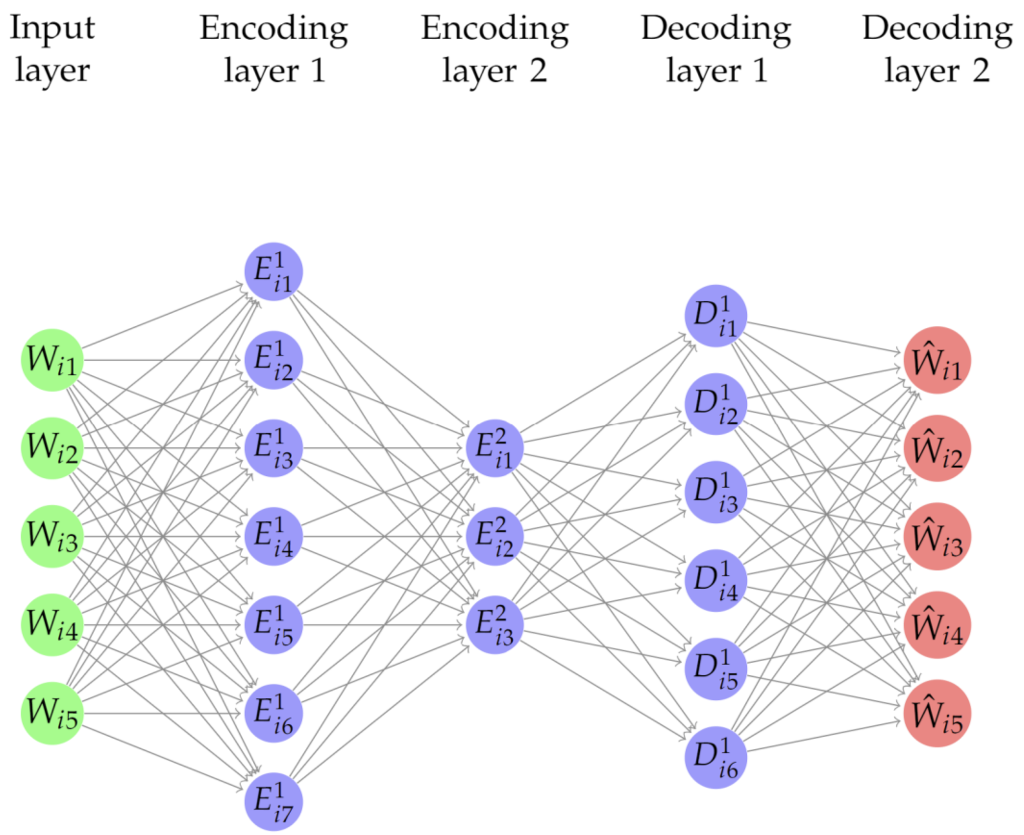
- For PCA, it also happens that the optimal is $A = C_K'$



Deep Encoders-Decoders (Auto-Encoders)

- Why only linear encoding and decoding functions
- Neural network-based encoders-decoders

$$W \overset{g_1}{\to} E_1 \overset{g_2}{\to} \ldots \overset{g_k}{\to} E_k \overset{f_1}{\to} D_1 \overset{f_2}{\to} \ldots \overset{f_m}{\to} D_m =: \widehat{W}$$



Deep Auto-Encoders

- Encoding part is an arbitrary function $e(W): \mathbb{R}^p \to \mathbb{R}^k$ with $k \ll p$
- Decoding part is an arbitrary function $d(X): \mathbb{R}^k \to \mathbb{R}^p$

- $X = e(W)$ is low dimensional "representation" or "embedding" of W

- Goal is to minimize some notion of "reconstruction error"

$$E_n\left[\text{loss}\Big(W, d\big(e(W)\big)\Big)\right]$$

From PCA to ICA

- The PCA reasoning lead to latent embeddings that are un-correlated
- Why not *independent?*
- Independent component analysis (ICA): find latent embeddings X that can reconstruct W but are jointly independent (not just uncorrelated)

- *Linear ICA:* find such latent embeddings that are also linear $X = C'W$
- Admits a clean solution with provable guarantees (Common'94)
- *Non-Linear ICA:* new literature on "disentangled representations"
- No clean solution (Locatello et al.'19); requires auxiliary information on latent factors X (e.g. Hyvarinen's work)

Variational Auto-Encoders

- So far mapping from W to X was deterministic

- More realistic: W is a stochastic projection of a low dimensional vector X onto a high-dimensional space

- In this case, we cannot reverse engineer X from W deterministically

- But we can maybe find a "posterior distribution" of X given W

Variational Auto-Encoders

- *Bottomline:* introduce randomness in the encoding part

- Introduce noise vector Z exogenously drawn (e.g. multivariate normal)
- $X = e(W, Z)$ is a low dimensional "sampled representation" of W, attempting to approximate the posterior distribution of X given W

- Goal is to minimize some regularized notion of "reconstruction error"

$$E_n\left[\mathrm{loss}\left(W, d\big(e(W,Z)\big)\right)\right]$$

Variational Auto-Encoders

- Typically, Z is multivariate standard normal and $e(W,Z)$ of the form
$$e(W,Z) = \mu(W) + \Sigma(W) \cdot Z$$

- $\mu(W)$: deterministic encoding of the mean of the posterior $X|W$
- $\Sigma(W)$: deterministic encoding of the variance of the posterior $X|W$

- The deterministic quantities $\mu(W)$ and $\Sigma(W)$ can be used as "embeddings" or engineered features on downstream tasks

General Embeddings

From Auto-Encoders to General Embeddings

- Auto-encoding (reconstruction objective) not the only objective to construct good embeddings
- *Generally:* consider many auxiliary tasks with different target outcomes A that resemble the task we want to solve
- *Goal:* find a common embedding $X \coloneqq e(W)$ that can be used to accomplish all tasks well, i.e. $\min_f E_n\left[loss\big(A, f(X)\big)\right] \ll small$, for all target outcomes A

- *Reasoning:* if the embedding carries sufficient information from W to be able to accomplish all these related tasks, then it should carry enough information to solve the task we care about

From Auto-Encoders to General Embeddings

- For text data, find an embeddings that perform well in many language tasks (e.g. Q&A, fill the gaps, predict next word)

- For image data, find embeddings that perform well in many vision tasks (e.g. classification, object detection etc.)

- Typically, we have much larger data sets for these auxiliary tasks than for the task at hand (e.g. web crawling data)
- We are essentially using these auxiliary data for more informed dimensionality reduction

Embeddings for Text Data

Word2vec

- We have a corpus of documents, containing a dictionary of n words
- Trivially we can embed words in n-dimensional one-hot encoding

$$e_j = (0, \dots, 1, \dots., 0)$$

- Too high-dimensional and not carrying “similarity” information
- Alternative: we want to find lower representations

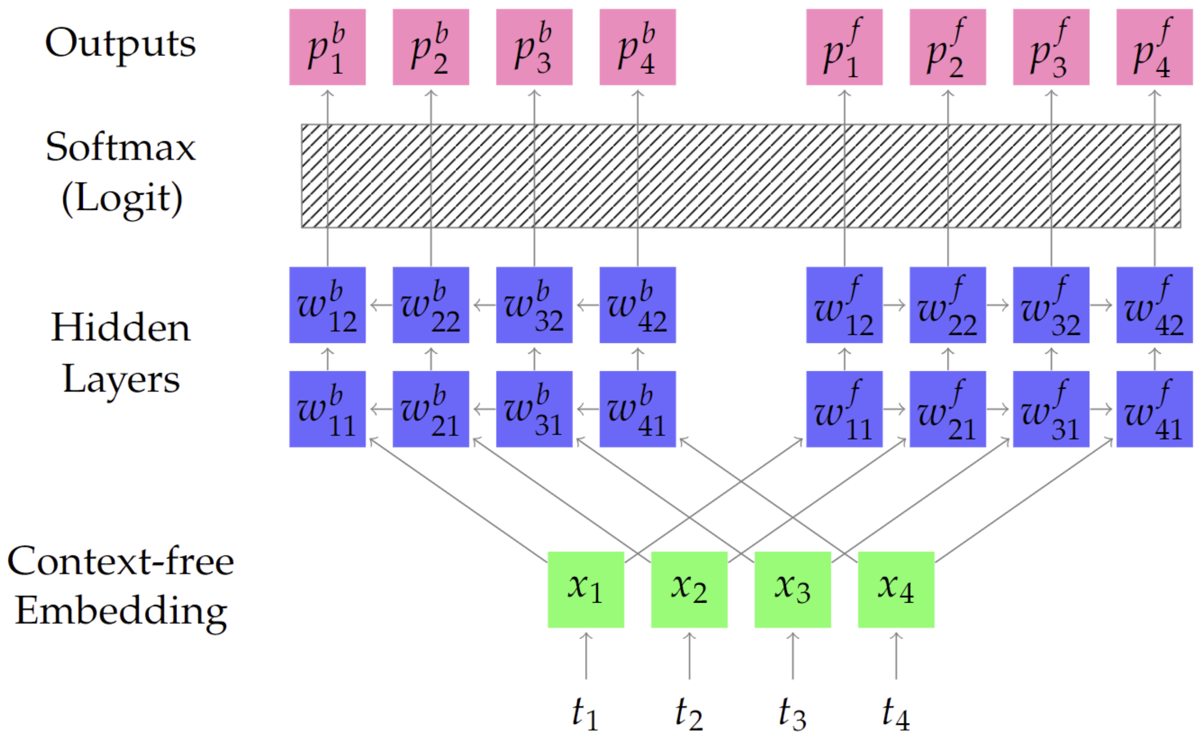
$$u_1, \dots, u_n$$

Word2vec

- Construct representations by solving a “fill-the-gap” text problem
- For each “middle word” s calculate average representation of K neighboring words $U_s = \frac{1}{K}\sum_{t\in N} u_t$
- Predict middle word equal to j given “context” U_s; logistic regression
$$p(j;\theta,u) = \Pr(T_s = j|\{T_t\}_{t\in N}) \propto \exp\left(\theta_j' U_s\right)$$
- Maximize over $\{\theta_j\}_{j=1}^{n}$ and $\{u_t\}_{t=1}^{K}$ the log-likelihood of observed data
$$\sum_s \log\big(p(T_s;\theta,u)\big)$$

Second Generation: ELMo

- Word2vec uses very rigid neighborhood model
- Distance from target word is not even incorporated in neighborhood embedding U_s
- ELMo addresses these issues by using Recurrent Neural Networks



Recurrent Neural Network

- A non-linear version of an auto-regressive model (Box-Jenkins)
- Nnet parses input "tokens" one-by-one; at each step t

non linearity

$$S_t = \sigma(AT_t + BS_{t-1} + c)$$

state

input token

previous state

$$y_t = \sigma(DS_t + e)$$

predicted outcome

state

Recurrent Neural Network

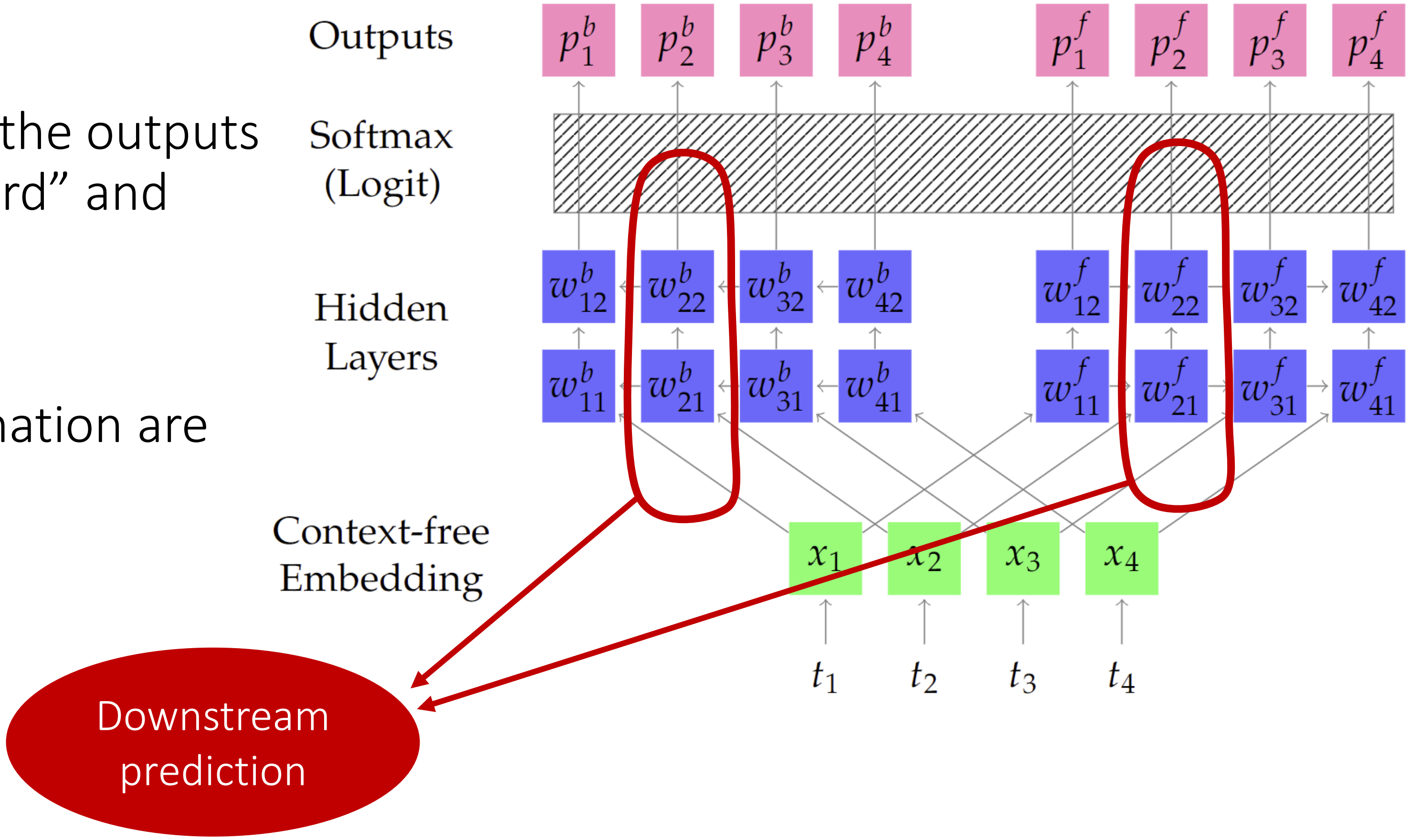
- A non-linear version of an auto-regressive model (Box-Jenkins)
- Nnet parses input “tokens” one-by-one; at each step t

$$S_t = \sigma(AT_t + BS_{t-1} + c)$$
$$y_t = \sigma(DS_t + e)$$

- When used for next word prediction problem it uses the actual “sequence” information; distance is encoded in the state
- Can capture long-range dependencies (albeit not-directly and unstable training)
- For this ELMo uses special RNN called a Long Short-Term Memory (LSTM) that enables more long-range “effects”

Embeddings from ELMo

- For each token in position k
- Consider a linear combination of the outputs of the neurons in the k-th "forward" and "backward" prediction column
- The weights on this linear combination are trained for the downstream task



Second Generation: BERT

- ELMo is very sequential and one-directional

- The context of a word in the prediction is either “previous words” or “subsequent words”
- Better to use context from both “directions” aka “bi-directional”

- Long-range dependencies in language are hard to capture (despite LSTM)
- We might want to create higher level “neighborhoods” that go beyond the local neighborhoods implicitly used in LSTM/RNN

Second Generation: BERT

- Better to use context from both “directions” aka “bi-directional”
- We might want to create higher level “neighborhoods” that go beyond the local neighborhoods implicitly used in LSTM/RNN
- We need the network to also learn “neighborhood structures”
- These “neighborhood structures” are known as “attention regions”

- When we calculate the “context” for predicting a word we want to take into account the average context of all the words in the attention region related to that word

Second Generation: BERT

- Better to use context from both “directions” aka “bi-directional”
- We might want to create higher level “neighborhoods” that go beyond the local neighborhoods implicitly used in LSTM/RNN

- Constructing such “trainable” attention regions associated with a word is what a “Transformer” architecture does

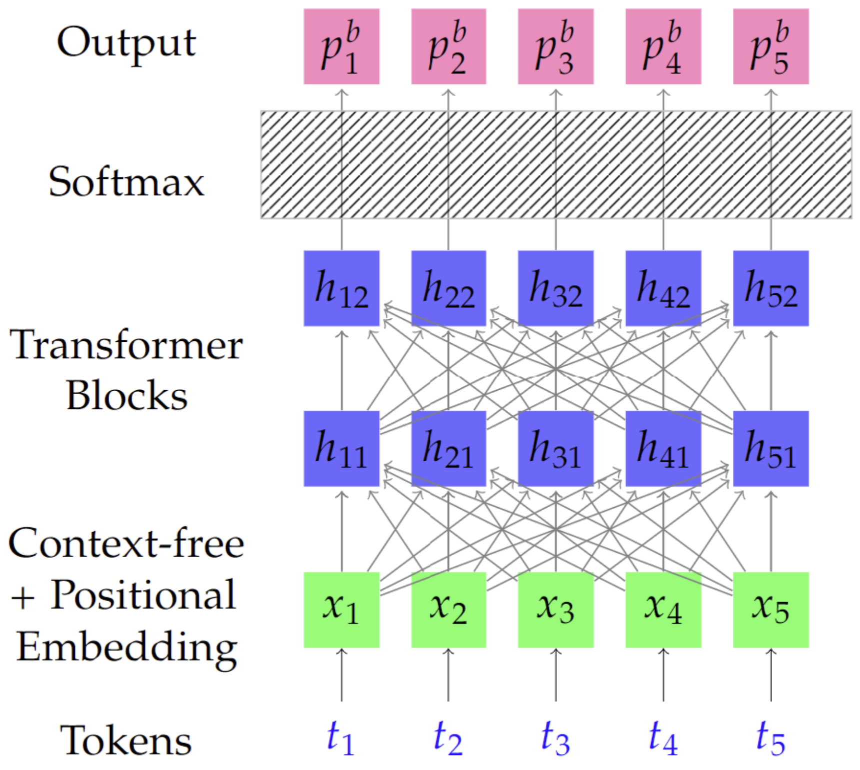
- So BERT uses **B**i-directional **E**ncoder **R**epresentations built with **T**ransformers

Second Generation: BERT

- The parameters are trained using two language tasks
- Mask: a random set of words in the document is masked and the goal is to predict them
- Pair: pairs of sentences are given and the goal is to predict if one sentence follows the other

Embeddings from BERT can be done in two ways:

- Outputs of the last few Transformer layers as features
- Fine tune whole network to target task; append a predictor at the end of the Transformer layers

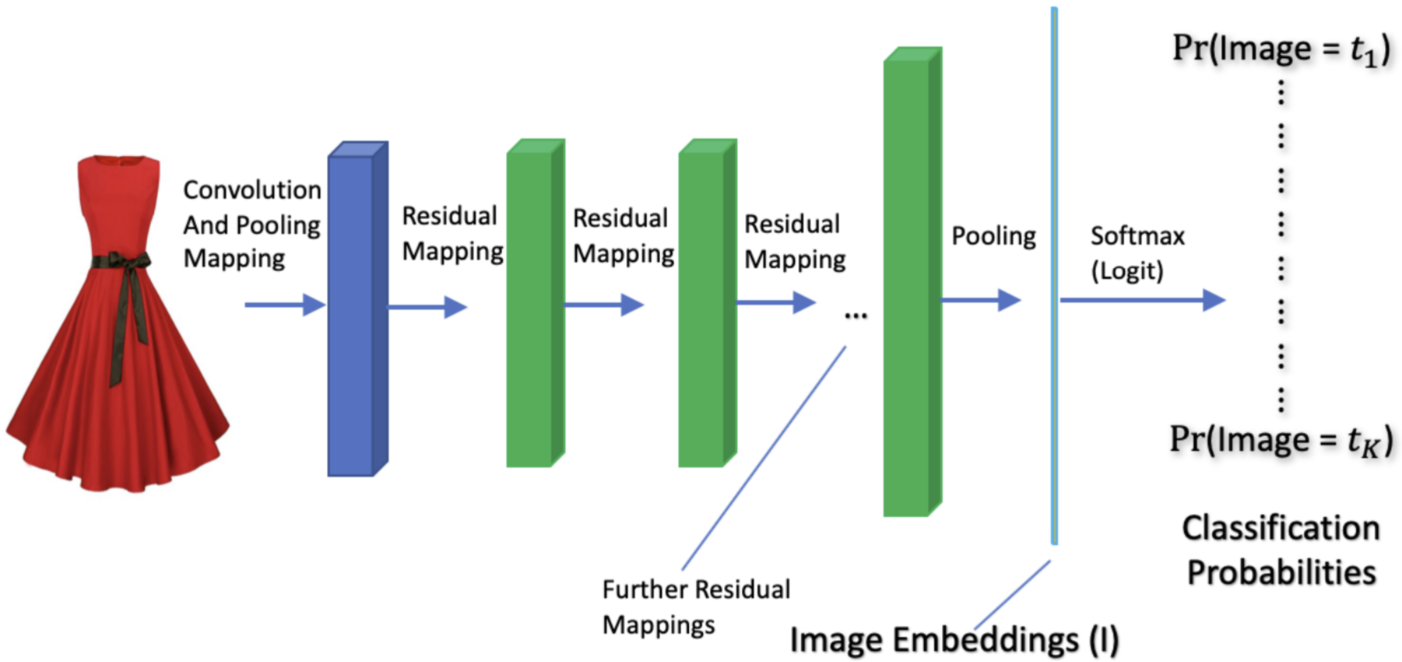


Third Generation: GPT (Generative Pre-Training) Family

- Ideas from the auto-regressive approach of ELMo (predict next words)
- With attention based encoding ideas in BERT, i.e. Transformers

Embeddings for Image Data

Classification Tasks and Convolutional Nets



ResNet: each block allows the input signal to also flow in-tact without a non-linearity

Embeddings for Price Prediction

Predicting prices from product characteristics at Amazon

Bajari et al. 2021, *Hedonic prices and quality adjusted price indices powered by AI*.

Nnet on top of embeddings ≈ 90%

Random Forest on embeddings ≈ 80%

Linear model of embeddings ≈ 70%

Linear model on simple features ≈ 40%