Deep Learning

4DV661

Regularization for Deep Learning

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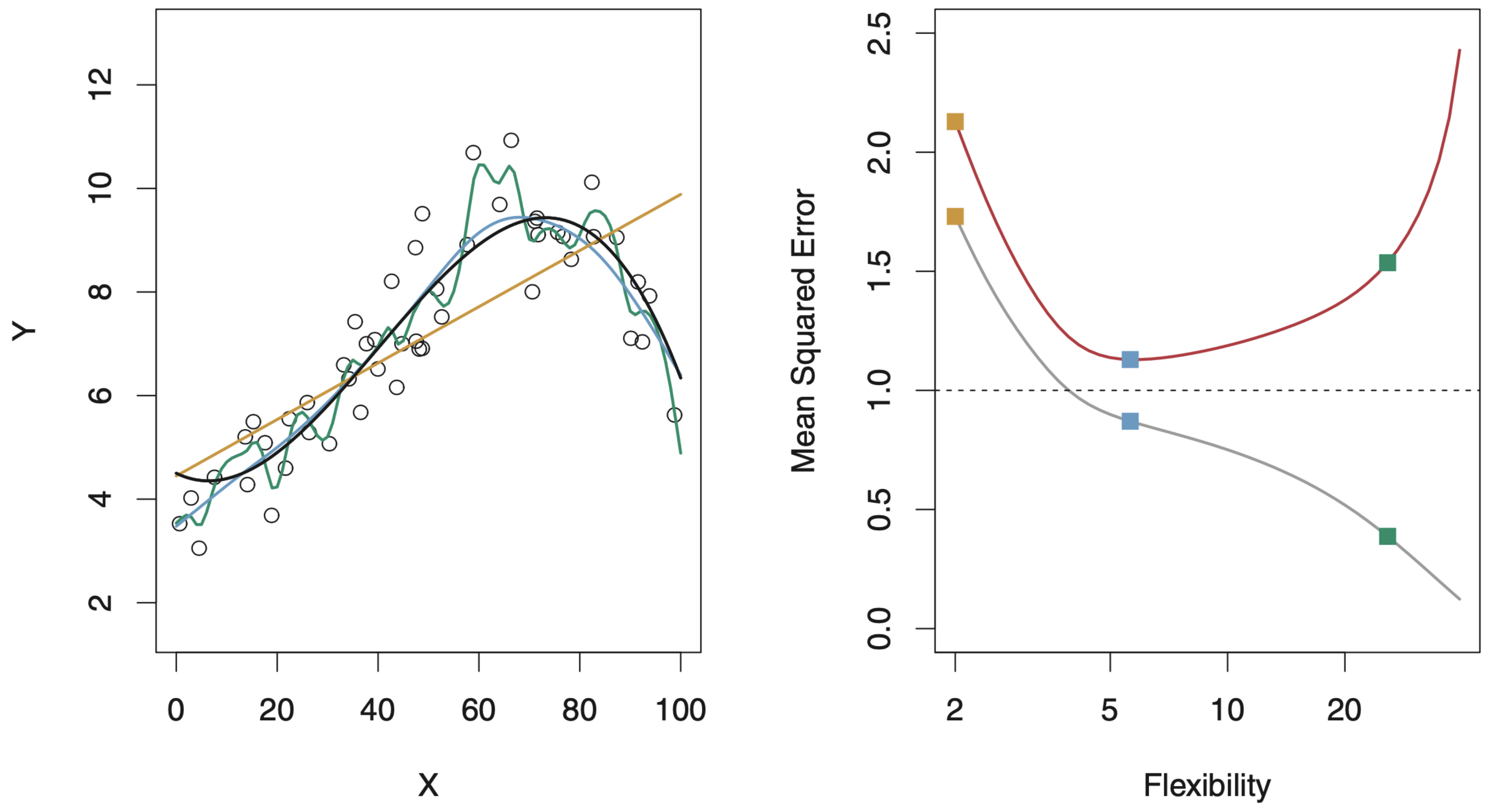
Course structure

1. Introduction
2. Applied Math Basics
3. Deep Feedforward Networks
4. Regularization for Deep Learning
5. Optimization for Training Deep Models
6. Convolutional Networks
7. Sequence Modeling: Recurrent and Recursive Nets
8. Practical Methodology
9. Applications

Problem of over-fitting



The Bias-Variance trade-off

- Variance of $\hat{f}$ refers to the amount by which $\hat{f}$ would change if we estimated it using different training data sets.
- Bias of $\hat{f}$ refers to the error that is introduced by approximating/simplifying a real-life problem.
- For any value x_0 the expected (squared) error is

$$E\left(y_0 - \hat{f}(x_0)\right)^2 = \mathrm{Var}(\hat{f}(x_0)) + [\mathrm{Bias}(\hat{f}(x_0))]^2 + \mathrm{Var}(\epsilon)$$

  - $\mathrm{Var}(\hat{f}(x_0)) = E(\hat{f}(x_0)^2) - E(\hat{f}(x_0))^2$ (definition of Var)
  - $\mathrm{Bias}(\hat{f}(x_0)) = E(\hat{f}(x_0)) - E(f(x_0)) = E(\hat{f}(x_0)) - f(x_0)$ (f is deterministic but unknown)

- More flexible models result in less bias but higher variance and vice versa.

The Bias-Variance trade-off (cont'd)

- The optimum flexibility level corresponds to the minimum test error optimizing the matching of the real-world with the model
- The relative rate of change of variance and bias determines whether the test MSE increases or decreases with model flexibility
  - the squared bias and variance may change at different rates
  - and we don't know the test MSE

- What does that mean for deep learning?

Motivation of Regularization

- (Sufficiently complex) deep learning models have basically no bias (perfect learner)
- This high flexibility leads too a high risk of overfitting (high variance)
- Regularization mitigates this problem by
  - Restricting the model flexibility
  - Restricting the training process
  - Adding new data (augmentation, later in the course)

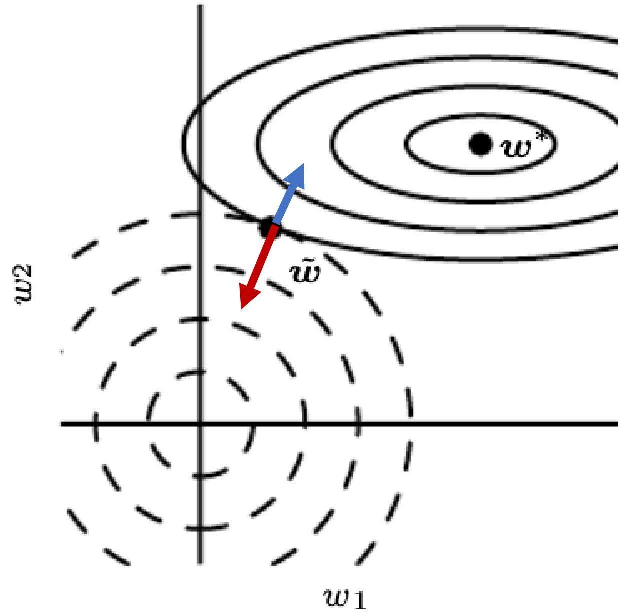
Agenda for today

- Parameter Norm Penalties
- Norm Penalties as Constraints
- Regularization and Under-Constrained Problems
- Dataset Augmentation
- Noise Robustness
- Semi-Supervised Learning
- Multitask Learning
- Early Stopping
- Bagging and Other Ensemble Methods
- Dropout
- Parameter Typing and Parameter Sharing
- Sparse Representations
- Adversarial Training
- Tangent Distance, Tangent Prop and Manifold, Tangent Classifier

Restricting the model flexibility

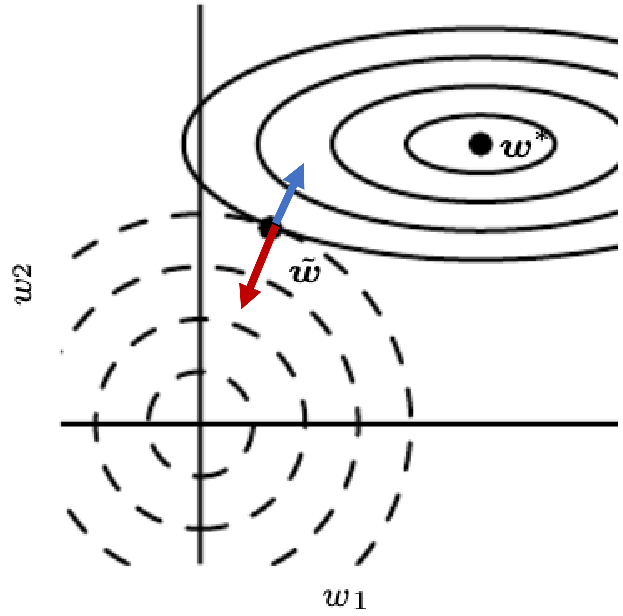
Restricting the training process

Parameter Norm Penalties



- The loss function has two components, i.e., the Original loss plus a Norm penalty function. We denote
  - the Original loss function $J(\boldsymbol{w})$ with $w*$ as the optimum
  - the Norm penalty function $\alpha\Omega(\boldsymbol{w})$ with Ω a norm of the weight vector and α a weight of this penalty
  - In the image, L2 norm, i.e., the squared length of the parameter vector
- Optimum $\tilde{w} \neq w*$ of the sum of both functions, i.e., $J(\boldsymbol{w})+\alpha\Omega(\boldsymbol{w})$ is minimum for $\boldsymbol{w}= \tilde{\boldsymbol{w}}$
  - $\nabla J(\tilde{\boldsymbol{w}}) \neq 0$, $J(\boldsymbol{w})$ gets smaller in the blue direction
  - $\nabla\Omega(\tilde{\boldsymbol{w}}) \neq 0$, $\Omega(\boldsymbol{w})$ gets smaller in the red direction
- Optimum can be found with gradient descent on the sum of both functions, i.e., $J(\boldsymbol{w})+\alpha\Omega(\boldsymbol{w})$
  - Iteratively adjust weights until $\nabla(J(\tilde{\boldsymbol{w}}) + \alpha\Omega(\tilde{\boldsymbol{w}})) \approx 0$

Norm Penalties as Constraints



- For a first try, substitute the penalty function $\alpha\Omega(\boldsymbol{w})$ with an equality constraint $\Omega(\boldsymbol{w}) = c$
  - So, we minimize $J(\boldsymbol{w})$ requiring the for norm $\Omega(\boldsymbol{w}) = c$
  - In the image, each dotted lines corresponds to the L2 norm with different values of c
- For the optimum $\widetilde{\boldsymbol{w}}$, the gradients of loss function $\nabla J(\widetilde{\boldsymbol{w}})$ and the norm function $\Omega(\boldsymbol{w})$ are parallel (both orthogonal to the tangent in $\widetilde{\boldsymbol{w}}$ on the contour of the loss and the norm functions)

$$\nabla J(\widetilde{\boldsymbol{w}}) = \lambda \nabla \Omega(\widetilde{\boldsymbol{w}}) \text{ and } \Omega(\widetilde{\boldsymbol{w}}) = c$$

- Parallel: there is only a scale factor λ of the gradients $\nabla J(\widetilde{\boldsymbol{w}})$ and $\nabla \Omega(\widetilde{\boldsymbol{w}})$ making these two vectors equivalent
  - Called the Lagrangian multiplier λ
  - Can be understood as a new variable to optimize for
- The condition can be formulated with the Lagrangian $\mathcal{L}$ and is gradient $\nabla \mathcal{L}$

$$\mathcal{L}(\boldsymbol{w}, \lambda) = J(\boldsymbol{w}) + \lambda(\Omega(\boldsymbol{w}) - c)$$
$$\nabla \mathcal{L}(\boldsymbol{w}, \lambda) = 0 \text{ and } \Omega(\widetilde{\boldsymbol{w}}) = c$$

- This looks like an unconstrained optimization problem. However, the solution is on saddle points of the Lagrangian, hence, gradient descent does not apply directly
- Still, we can transform the problem such that the solution is a minimum of the transformed problem, e.g., minimize the (squared) magnitude of the gradient of the Lagrangian (≥ 0).

Norm Penalties as Constraints (cont'd)

- We have transformed an equality-constrained minimization problem in an unconstrained optimization problem, but
- For regularization, we face an inequality constraint: $\Omega(\boldsymbol{w}) \leq c$
- This can easily be transformed into an equality constraint using a slack variable s (adding a new variable to optimize for)

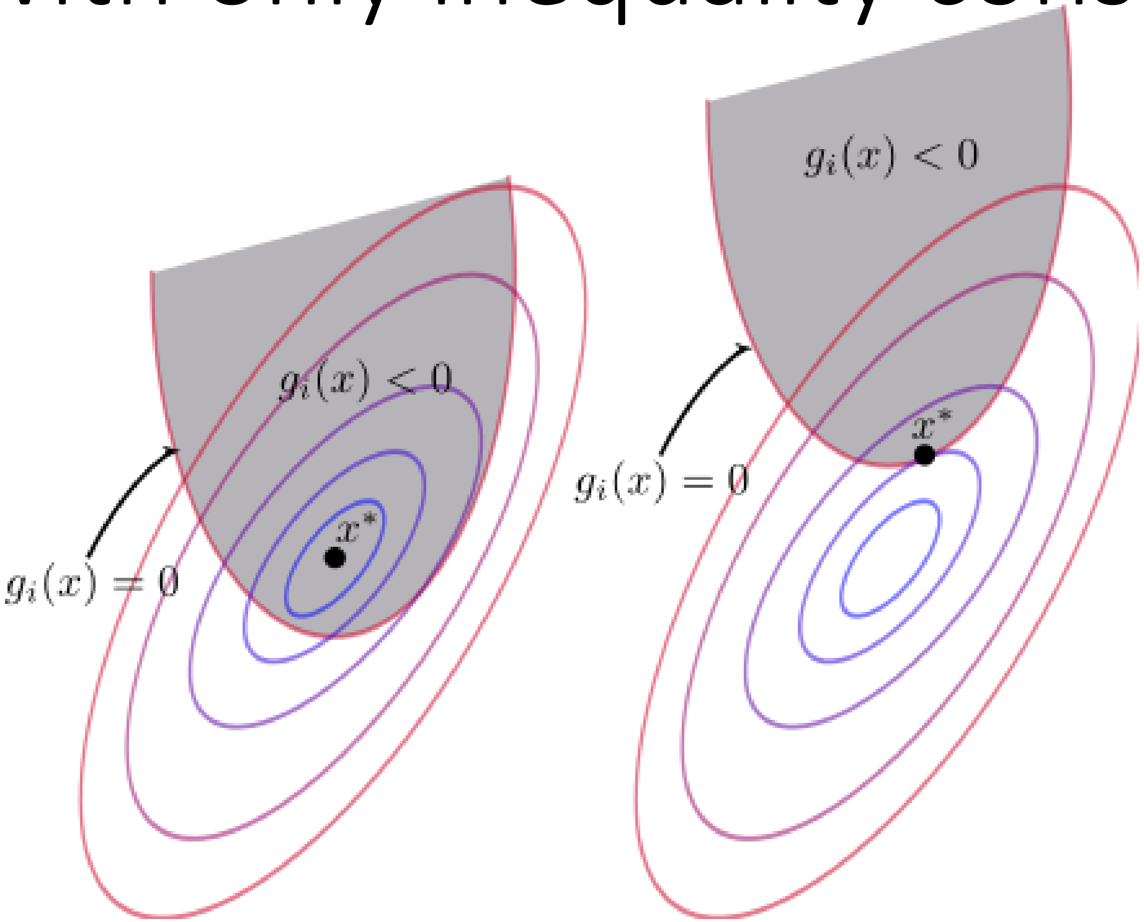
$$\Omega(\boldsymbol{w}) + s^2 = c.$$

- Changes the Lagrangian and the condition:

$$\mathcal{L}(\boldsymbol{w}, \lambda, s) = J(\boldsymbol{w}) + \lambda(\Omega(\boldsymbol{w}) + s^2 - c)$$
$$\nabla\, \mathcal{L}(\boldsymbol{w}, \lambda, s) = 0 \text{ and } \Omega(\boldsymbol{w}) + s^2 = c$$

- Solution by reduction to an unconstraint case and an equality constraint case disregarding the slack with the Karush–Kuhn–Tucker (KKT) approach

KKT cases with only inequality constraints $g(x)$



3a) Solution is equal to the unconstraint case (constraint is inactive)

3b) Solution is equal to the equality constraint case (constraint is active)

https://en.wikipedia.org/wiki/Karush%E2%80%93Kuhn%E2%80%93Tucker_conditions

Norm regularization in Tensorflow

Practical hints:

- Given a regression equation y=Wx+b, where x is the input, W the weights matrix and b the bias vector.
  - Kernel regularizer tries to reduce the weights W (excluding bias).
  - Bias regularizer tries to reduce the biases b.
  - Activity regularizer tries to reduce the layer's output y, thus, it will adjust the weights and the bias so Wx+b is constrained.
- If you have no idea about the function that you wish to model, only use the Kernel Regularizer
  - since a large enough network can still model your function even if the regularizations on the weights are big.
- If you want the output function to pass through (or have an intercept closer to) the origin, use the Bias Regularizer.
- If you want the output to be smaller (or closer to 0), use the Activity Regularizer.

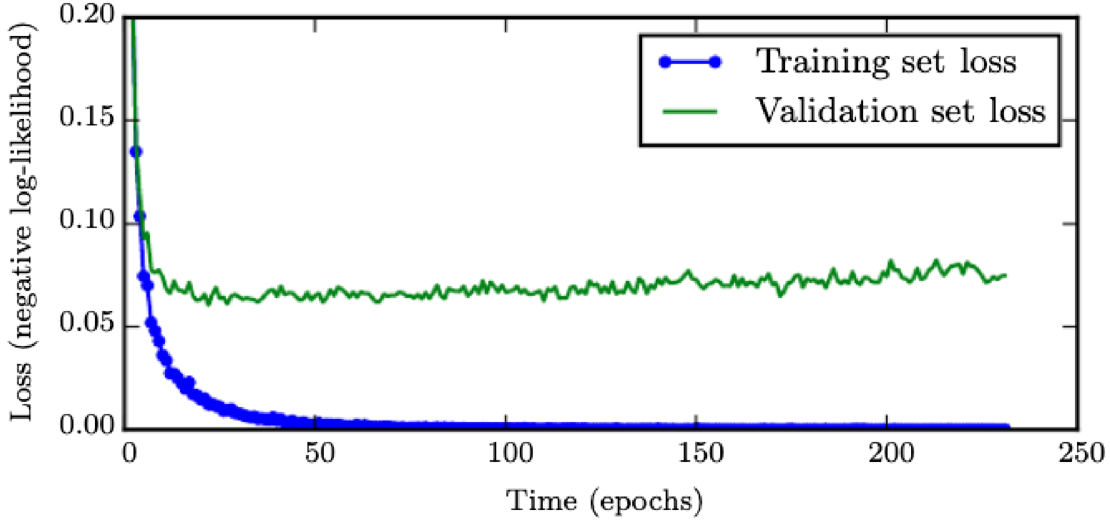
Norm Regularization in Tensorflow (cont'd)

- $L1$ versus $L2$ loss (not to be confused with the networks loss function).
  - $L2$ loss is defined as $|w|_2 = \sqrt{\sum(w_i)^2}$
  - $L1$ loss is defined as $|w|_1 = \sum w_i$.
- The gradient of
  - $L2$ will be: $2w$
    $L1$ will be: $sign(w)$
- In Norm Regularization, for each gradient update with a learning rate of ε and a weight decay of α, using $L2$ loss, the weights will be subtracted by $\varepsilon\alpha \cdot w$, while in $L1$ loss they will be subtracted by $\varepsilon\alpha \cdot sign(w)$.
- The effect of $L2$ loss on the weights is a reduction of large components in the weight matrix while $L1$ loss will make the weights matrix sparse, with many zero values.
  - The same applies on the bias and output respectively using the bias and activity regularizer.

Demo

- Notebooks https://github.com/WelfLowe/Public-ML-Notebooks/
- Check: Regularization of linear regression with norms and constraints
- For equality constraint optimization, check: Constraint Optimization (this is FYI about the approach; it is not a regularization method)

Early stopping



- Check training and validation loss under training
- Continue minimizing the training loss over the epochs
- However, keep the (parameters of the) model with the lowest validation loss
- Can be interpreted as hyper-parameter (number of epochs) learning

Early stopping (cont’d)

- Requires a validation set, which means some training data is not shown to the optimizer for deriving (gradients of) the model (parameters).
  - Yet the final model is not independent of validation data
  - Therefore, distinguish validation from test data
  - Use cross-validation and -testing
- Needs additional data, processing and memory recourses
- Otherwise, its an unobtrusive form of regularization
  - No negative effect
  - No changes to the optimization goal
  - Possibly used together with other regularization strategies

Bagging/Ensemble methods – idea

- Bagging (bootstrap aggregation): construct k different datasets
  - Each bag contains the same number of data point,
  - constructed by sampling with repetition from the original dataset,
    - not necessary a fair sample
    - you might, e.g., choose to oversample the minority class
  - with high probability, each bag is missing some of the examples (1/3 is OOB)
- Ensemble: construct k different models
  - train k different models separately,
  - different models will usually not make all the same errors on the test set
- Model aggregation: models' mode (classification) or mean (regression) sets the output for test examples
  - Stacking: aggregation by yet another ML model

Effect of Bagging/Ensemble methods

- Each of the k models (for the k bags) makes an error ϵ_i,
- Assume ϵ_i are drawn from a zero-mean multivariate normal distribution with
  - variances $Var[\epsilon_i]$ =$\mathrm{E}[\epsilon_i^2] = \frac{1}{k}\sum \epsilon_i^2 = v$ and covariances $Cov[\epsilon_i \epsilon_j] = \mathrm{E}[\epsilon_i \epsilon_j] = \frac{1}{k}\sum \epsilon_i \epsilon_j = c$.
- The expected (squared) error of the ensemble is $\frac{1}{k}\sum \epsilon_i$ and the expectation of the squared error is

$$\mathbb{E}\left[\left(\frac{1}{k}\sum_i \epsilon_i\right)^2\right] = \frac{1}{k^2}\mathbb{E}\left[\sum_i \left(\epsilon_i^2 + \sum_{j\neq i} \epsilon_i \epsilon_j\right)\right]$$
$$= \frac{1}{k}v + \frac{k-1}{k}c.$$

- Perfectly correlated errors between the models (c=v): Expectation of $MSE = v$, i.e., no effect.
- Perfectly uncorrelated errors between the models (c=0): Expectation of $MSE = \frac{1}{k}v$, i.e., the error is inverse proportional to the number of models.
- Truth somewhere in between

Proof hints

- Total variance:

$$\sum_{i=1}^{k}\sum_{j=1}^{k}\mathrm{Cov}(e_i,e_j)=\sum_{i=1}^{k}\mathrm{Var}(e_i)+\sum_{i\neq j}\mathrm{Cov}(e_i,e_j)=k\sigma^2+k(k-1)c.$$

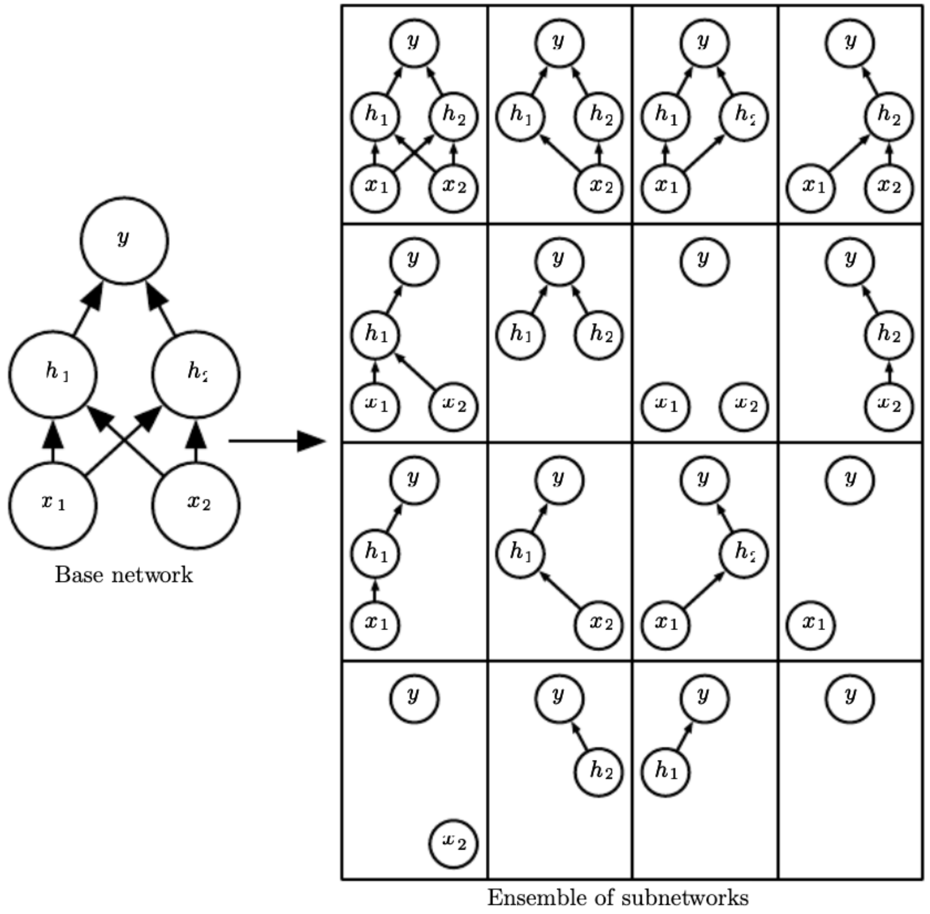
- Simplification of the expected squared error:

$$\left(\sum_i a_i\right)^2=\sum_i a_i^2+2\sum_{i<j}a_ia_j$$

Bagging in Deep Learning

- Bootstrap: choose mini batches, i.e., samples from the original dataset, in each epoch
  - As the name suggests: mini batches are smaller than the full training set
- Aggregation: take the minimum weights from the current epoch as initialization for the next epoch (optimized with a new mini batch)
  - However, models are not learned independently
  - Resemble boosting in this respect

Dropout



- Can be interpreted as a special ensemble method
- Mask vector μ specifies which units to include
- Cost function $J(\theta, \mu)$ of the cost of the model defined by parameters θ and mask μ.
- Dropout training minimize the expectation $\mathrm{E}_{\mu}[J(\theta, \mu)]$.

Dropout Analogy to Ensemble

- Ensemble accumulates the votes from all its members
- Assume that (each) model i outputs a probability distribution
- Ensemble averages these distributions

$$\frac{1}{k}\sum_{i=1}^{k} p^{(i)}(y \mid \boldsymbol{x})$$

- In the case of dropout, $p(\mu)$ is probability of mask μ at training time

$$\sum_{\boldsymbol{\mu}} p(\boldsymbol{\mu}) p(y \mid \boldsymbol{x}, \boldsymbol{\mu})$$

Assignment 4

- Read Chapter 8 (54 pages): Optimization for Training Deep Models
- Check out, understand, and reimplement the Jupyter notebook: “Regularization of linear regression with norms and constraints.pdf” (in MyMoodle). Implement regularization with the
  - norm penalty using the L1 or L2 norm and
  - norm inequality constraint using the L1 or L2 norm and
- All implementation in Python and explain what you have done.

- Deadline: 2025-04-29 (before the next lecture)