Regularization

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Regularization

Goal: Reduce generalization error

Strategies:

- Constraints on parameter values
  e.g. try to keep parameters from being too small/large
- Preferences for simpler models
- Guidance for underspecified problems
- Combine multiple hypotheses (ensemble methods)

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Parameter norm penalties

Attempt to limit capacity

$$\tilde{J}(\theta \mid X, y) = \underbrace{J(\theta \mid X, y)}_{\substack{\text{loss/} \\ \text{objective} \\ \text{function}}} + \underbrace{\alpha\Omega(\theta)}_{\substack{\text{penalty} \\ \text{depends} \\ \text{on model } \theta}}$$

- $\alpha \in [0, \text{inf})$ is user settable
- Common to use a L^p norm for $\Omega(\Theta)$
- Model Θ comprised of weights w; $\tilde{J}(w|X, y)$ is equivalent

Remember L^p, or $\|x\|_p = \left(\sum_i |x_i|^p\right)^{1/p}$ (Goodfellow et al. 2.5)

Parameter norm penalties

- Common to ignore bias
  - only shifts position
  - penalizing frequently results in underfitting
- Separate α per layer is possible, but…
  - complicates hyperparameter search
  - reasonable to use global α.

Parameter norm penalties

We will discuss two:

- L2 – Causes weights to get smaller
  - Shrinkage proportional to weight
  - AKA "weight decay"
- L1 – Makes weight vector "sparse"
  - Pulls weights towards zero by constant factors

L^2 penalty

- Weight decay* penalty $\Omega(\theta) = \alpha_0 \frac{1}{2} w^T w$

$$\tilde{J}(\theta \mid X, y) = J(\theta \mid X, y) + \alpha\Omega(\theta) \quad \alpha = \frac{1}{2}\alpha_0$$
$$= J(\theta \mid X, y) + \alpha w^T w$$

- $\nabla_w \left(\alpha_0 \frac{1}{2} w^T w \right) = \alpha_0 \frac{2}{2} w$, so

$$\nabla_w \tilde{J}(\theta \mid X, y) = \nabla_w J(\theta \mid X, y) + \alpha_0 w$$

* Also known as ridge regression & Tikhonov regularization

L^2 penalty

- Consider weight update

$$w \leftarrow w - \epsilon \nabla_w \tilde{J}(\theta \mid X, y)$$

$$\begin{aligned} & w - \epsilon \nabla_w \tilde{J}(\theta \mid X, y) = \\ & w - \epsilon \left(\nabla_w J(\theta \mid X, y) + \alpha_0 w \right) = \\ & w - \epsilon \alpha_0 w - \epsilon \nabla_w J(\theta \mid X, y) = \\ & (1 - \epsilon \alpha_0) w - \epsilon \nabla_w J(\theta \mid X, y) \end{aligned}$$

$$w \leftarrow (1 - \epsilon \alpha_0) w - \epsilon \nabla_w J(\theta \mid X, y)$$

Tends to shrink weights (with appropriate αε)

L^2 penalty

- For a quadratic penalty (e.g. regression), this has the affect of scaling directions by the eigen-values of the Hessian matrix

oh, oh…
rabbit hole

British Postal Service, Graham Baker-Smith 2015

Hessian matrix – H

$$g : \mathbb{R}^m \rightarrow \mathbb{R}^n$$

$$\left[\frac{\partial y}{\partial x}\right] = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \cdots & \frac{\partial y_1}{\partial x_M} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & & \frac{\partial y_2}{\partial x_M} \\ \frac{\partial y_3}{\partial x_1} & \frac{\partial y_3}{\partial x_2} & & \frac{\partial y_1}{\partial x_M} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial y_N}{\partial x_1} & \frac{\partial y_N}{\partial x_2} & \cdots & \frac{\partial y_N}{\partial x_M} \end{bmatrix}$$

Jacobian (saw earlier)

$$\left[\frac{\partial^2 y}{\partial x_i \partial x_j}\right] = \begin{bmatrix} \frac{\partial^2 y_1}{\partial x_1^2} & \frac{\partial^2 y_1}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 y_1}{\partial x_1 \partial x_M} \\ \frac{\partial^2 y_2}{\partial x_2 \partial x_1} & \frac{\partial^2 y_2}{\partial x_2^2} & & \frac{\partial^2 y_2}{\partial x_2 \partial x_M} \\ \frac{\partial^2 y_3}{\partial x_3 \partial x_1} & \frac{\partial^2 y_3}{\partial x_3 \partial x_2} & & \frac{\partial^2 y_1}{\partial x_3 \partial x_M} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial^2 y_N}{\partial x_M \partial x_1} & \frac{\partial^2 y_N}{\partial x_M \partial x_2} & \cdots & \frac{\partial^2 y_N}{\partial x_M^2} \end{bmatrix}$$

Hessian is 2nd partial derivative

Goodall et al. 4.3.1

Hessian matrix

So why do we care…

- Sometimes used in gradient descent
- Provides an explanation for what's happening with L^2 penalty.

L^2 penalty

Consider approximation near optimal point without regularization: w^*

$$\hat{J}(w) = \underbrace{J(w^*)}_{\substack{\text{best possible} \\ \text{parameters} \\ \text{w/o regularization}}} + \underbrace{\frac{1}{2}(w-w^*)^T H(w-w^*)}_{\substack{\text{scale distance from optimal} \\ \text{by rate of change}}}$$

L^2 penalty

- $w \in R^2$
- w^* optimal w/o penalty
- w_2 has more affect on J(w)
- $\tilde{w}$ equilibrium between loss and penalty

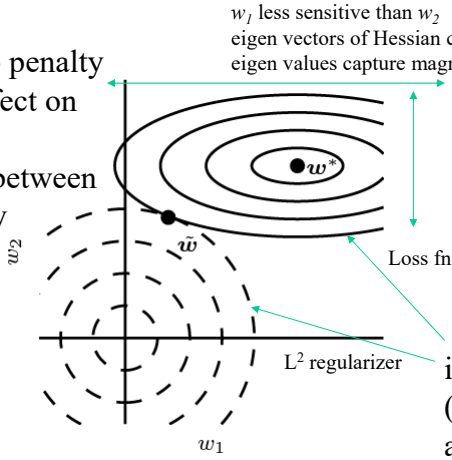


Fig. 7.1 Goodall et al.

L1 penalty

- L1 penalty $\Omega(\theta) = \sum_i |w_i|$

$$\tilde{J}(\theta \mid X, y) = J(\theta \mid X, y) + \alpha\Omega(\theta)$$
$$= J(\theta \mid X, y) + \alpha \sum_i |w_i|$$

- Gradient

$$\nabla_w \tilde{J}(\theta \mid X, y) = \nabla_w J(\theta \mid X, y) + \alpha \text{sign}(w)$$

L1 penalty

- As weights are pulled towards zero, fewer will be active.
- Leads to more zeros, or a *sparse representation*
- Can be thought of as a type of feature selection and is used in one popular algorithm (LASSO).

Keras and L1/L2 penalties

Penalties are specified when constructing layers, example

```
from keras import regularizers
# other imports…

Dense(N, kernel_regularizer=regularizers.l2(α), …)
OR
Dense(N, kernel_regularizer=regularizers.l1(α), …)
```

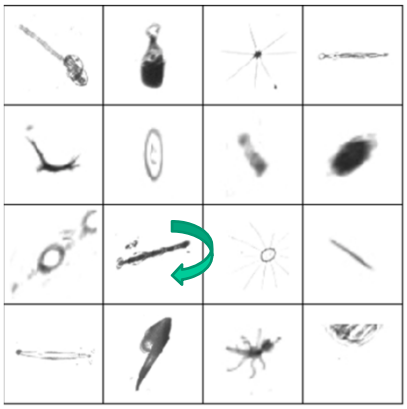
Starting point for α? Perhaps 0.01

Dataset augmentation

- We can improve classifiers by increasing training data.
- Data are expensive (most of the time)
- Solution:

Dataset augmentation

- Primary application: classification tasks
- Basic idea
  - Transform inputs slightly
  - Frequently used in image processing
  - Transforms such as rotation, scale, shift



Plankton classification challenge http://www.datasciencebowl.com

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Dataset augmentation for audio

- Can be a bit harder
- Some strategies
  - vocal tract length perturbation (Jaitly & Hinton 2013)
  - stretching, compressing
  - enhancements, e.g. adding noise (Prisyach et al. 2015)
    (small perturbations of inputs can be shown to be equivalent to L^p penalties on weights)

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Noise robustness

- We have already seen input perturbation (dataset augmentation)
- We can add noise to other parts of the network
- One approach is to add noise to the weights, e.g. $N(0, \eta \mathrm{I})$

Weight perturbation interpretation

- Bayesian view: Weight values have a distribution and we are drawing from these
- With MSE cost functions and small variance (η), perturbation $\equiv$ to adding penalty $\|\nabla_w \hat{y}(x)\|^2$
- Encourages optimization to find areas in parameter space where small weight changes have little influence on output (flat valleys in loss space)

Label Smoothing

- Inject noise at output targets
- Maximizing $\log P(y|x)$ can lead to overfitting.
- Common to inject noise onto output target.
- Rob Peter to pay Paul…
  - one hot target $1-\epsilon$
  - others $\frac{\epsilon}{N-1}$

use standard softmax cost function with cross-entropy

Multitask learning

- Learn different functions from same data
- Pool portions of the network to learn common things
- Decreases generalization error

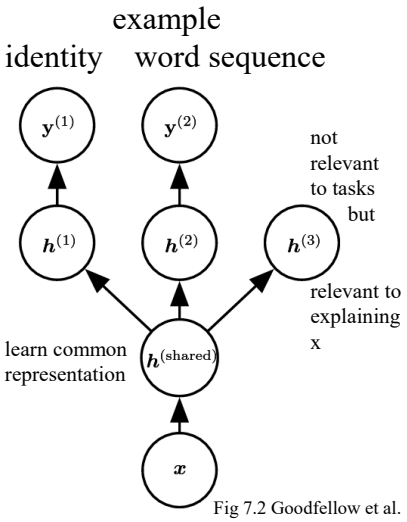
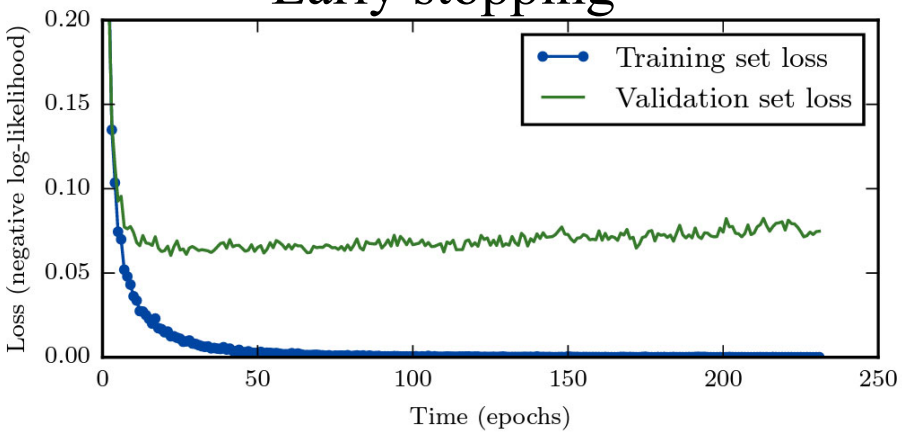


Fig 7.2 Goodfellow et al.

Early stopping



- Use other data to determine when to stop

Early stopping

Set loss to ∞
while we still have patience
    Update model Θ by n steps
    Check new loss on separate data
    If new loss < loss:
        store new loss, model, iteration
    decrease patience
return best model

see Alg. 7.1 for details

Early stopping

- Variants exist
- One such variant:

  Create new model and retrain for the same number of steps up to stop with *all* data.

  Alg. 7.2

Parameter tying

- Similar to multitask learning
- Learn two similar functions f_A and f_B with parameters Θ_A and Θ_B.
- Assume it makes sense for $w_A \in \theta_A$ and $w_B \in \theta_B$ to have similar weights

  key idea: similar features may be used

Parameter tying

- Force weights to be similar with penalty, e.g. L2 penalty:

$$\Omega\left(w^{(A)}, w^{(B)}\right) = \left|\left|w^{(A)} - w^{(B)}\right|\right|_2^2$$

Parameter sharing

- Similar idea, weights in nodes are learning similar things. e.g. a feature in two networks A and B.
- Differs in that the *same* set of weights are used in both networks.

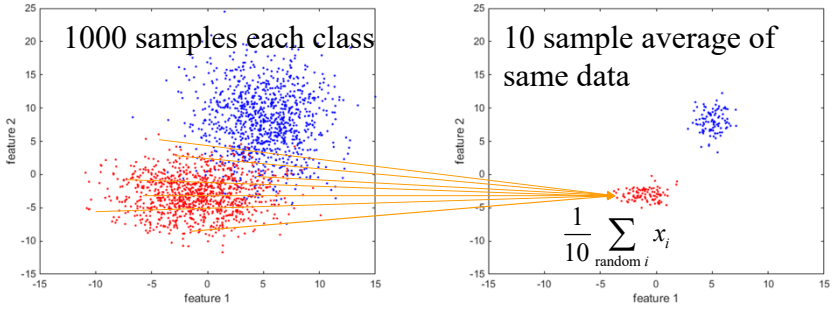
Sparse representation

- L1 penalties cause weights to tend towards zero, giving a *sparse parameterization*.
- *Sparse representations* occur when many of the *parameters* tend towards zero.
- Can be accomplished with a L1 penalty on layer outputs: $\alpha\Omega(h) = \alpha\frac{1}{m}\sum_i h^{(i)}$, other methods exist

Ensemble methods

- We know that models make mistakes.
- We hope that the error is randomly distributed…
- If so, averaging model outputs should reduce the noise.

Why this works
Example averaging features
(as opposed to model outputs)



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Bootstrap aggregation
Bagging, or model aggregation

- Ensemble method
- Train multiple networks
  - Usually with different data
  - Due to randomness in neural nets, can be done with same data
- Classify and vote/average output

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Bagging expected variance

- Suppose k models m_1, m_2, …, m_k
  - Assume errors $\epsilon_i \sim n(0, v)$
  - It follows that $\mathrm{E}[(\epsilon_i - 0)^2) = E[\epsilon_i^2] = v$
- Suppose covariances of errors are
  $$E[(\epsilon_i - 0)(\epsilon_j - 0)] = E[\epsilon_i \epsilon_j] = c$$
- Consider the variance of the mean error across models: $\mathrm{E}\left[\left(\frac{1}{k}\sum_i(\epsilon_i - 0)^2\right)\right]$

Expected bagging variance

$$E\left[\sum_i\left(\frac{1}{k}(\epsilon_i - 0)\right)^2\right]$$
$$= \frac{1}{k^2}E\left[\left(\sum_i \epsilon_i\right)^2\right]$$
$$= \frac{1}{k^2}E\left[\left(\epsilon_1 + \epsilon_2 + \epsilon_2 + \cdots + \epsilon_k\right)^2\right]$$
$$= \frac{1}{k^2}E\left[\left(\epsilon_1^2 + \epsilon_1\epsilon_2 + \cdots + \epsilon_1\epsilon_k\right) + \left(\epsilon_2\epsilon_1 + \epsilon_2^2 + \epsilon_2\epsilon_3 + \cdots + \epsilon_2\epsilon_k\right) + \cdots + \left(\cdots + \epsilon_{k-1}\epsilon_k + \epsilon_k^2\right)\right]$$
$$= \frac{1}{k^2}E\left[\sum_i\left(\epsilon_i^2 + \sum_{i \neq j}\epsilon_i\epsilon_j\right)\right]$$

Expected bagging variance

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

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

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

$$= \frac{1}{k^2}\left(\sum_i v + \sum_i \sum_{i \neq j} c\right) \quad \text{as } E[\epsilon_i] = v, E[\epsilon_i \epsilon_j] = c$$

$$= \frac{1}{k^2}\left(kv + k(k-1)c\right) = \frac{1}{k} v + \frac{k-1}{k} c$$

Expected bagging variance

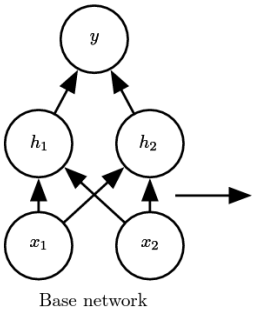
$$E\left[\left(\frac{1}{k}\sum_i (\epsilon_i - 0)^2\right)\right] = \frac{1}{k} v + \frac{k-1}{k} c = \frac{v + (k-1)c}{k}$$

- What if errors are perfectly correlated?
  - Then we would expect $E[\epsilon_i \epsilon_j] = v$ and would be back where we started with a mean variance of v.
- If errors are uncorrelated, $E[\epsilon_i \epsilon_j] = 0$, we have shrunk variance by a factor of k
- As we vary the data or models, we expect somewhere between the extremes, reducing the variance.

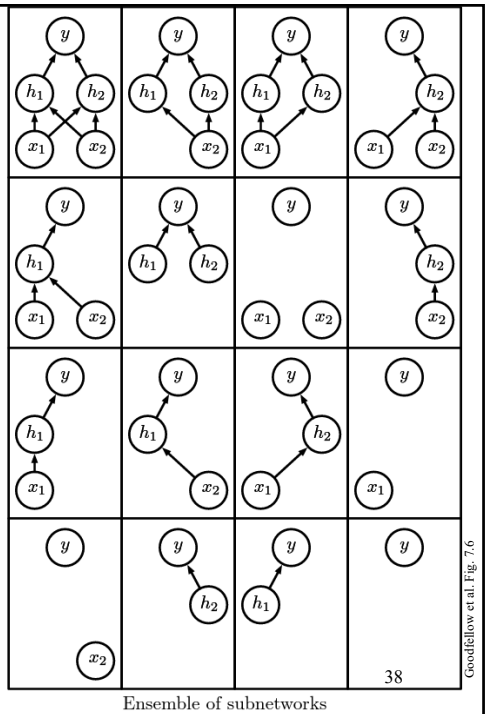
Dropout

- Related to bootstrap aggregation
- Builds implicitly different models as opposed to explicit ones

Dropout



Base network



Ensemble of subnetworks

Each training example uses a sampled subnet

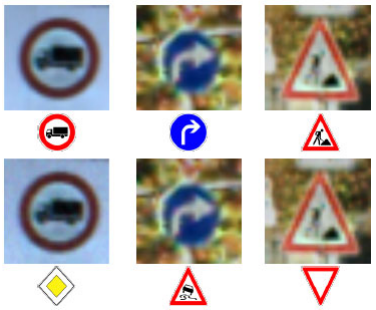
Goodfellow et al. Fig. 7.6

Dropout

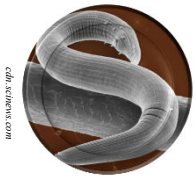
- Each sampled model shares weights with all other models
- Prediction weights each unit's output by probability of it being dropped
  (know as the weight scaling inference rule)

Adversarial training

Sometimes, moving away from an example in feature space can cause radical changes in labeling



Papernot et al. 2017 ACM Conf Comp Sec



Uh-oh…

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Moves away from the cost gradient can accomplish this:

Goodfellow et al. Fig. 7.8

$\boldsymbol{x}$	$\text{sign}(\nabla_{\boldsymbol{x}} J(\boldsymbol{\theta}, \boldsymbol{x}, y))$	$\boldsymbol{x} + \epsilon\,\text{sign}(\nabla_{\boldsymbol{x}} J(\boldsymbol{\theta}, \boldsymbol{x}, y))$
$y =$"panda" w/ 57.7% confidence	"nematode" w/ 8.2% confidence	"gibbon" w/ 99.3% confidence

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Adversarial training

- Specific type of dataset augmentation
- Find examples close to the data that have different predicted labels
- Train on them with the correct label
  - If label is not verified, it is called a virtual adversarial example