#### PGMO Lecture: Vision, Learning and Optimization 8. Learning

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## Introduction



- So far we have considereded mainly convex models based on the total variation, which however only served as a crude approximation to the true image statistics.
- ▶ In this chapter we will discuss methods to learn better variational models from data.
- We will start be learning just the regularization parameter but then will also learn filters and potential functions.
- Finally, we will also consider deep-learning inspired architectures that achieve state-of-the-art performance.

#### Overview

#### Parameter learning in variational models

The Fields of Experts model

Early stopping

Total Deep Variation

Learning with graphical models

#### Learning regularization parameters

▶ In [Kunisch, P. '12] we considered a weighted sum of  $\ell_1$  regularizers:

$$\mathcal{R}(u) = \sum_{k=1}^{N_{\mathcal{K}}} \vartheta_k \left\| \mathcal{K}_k u \right\|_1 = \sum_{k=1}^{N_{\mathcal{K}}} \sum_{i,j} \vartheta_k |(\mathcal{K}_k u)_{i,j}|,$$

where  $K_k$  are linear operators and  $\vartheta_k \ge 0$  are the regularization weights.

- Can be see as a generalization of the total variation
- ► Usually, we restrict the linear operators to small convolution kernels  $f_k$  with the property that  $K_k u \Leftrightarrow f_k * u$
- From JPEG compression, it is known that images have a sparse representation in terms of DCT basis functions.



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- In machine learning a popular approach is empirical risk minimization adopting a loss function.
- We assume we have given training data  $(f_s, g_s)_{s=1}^S$  consisting of noisy observations  $f_s$  and ground truth reconstructions  $g_s$ .
- Applying this idea to our image reconstruction problems leads to a bilevel optimization problem [Kunisch, P. '12]

$$\begin{cases} \min_{\vartheta \ge 0} \frac{1}{2} \sum_{s=1}^{S} \|u_s(\vartheta) - g_s\|_2^2 \\ \text{s.t. } u_s(\vartheta) = \arg\min_{u} \sum_{k=1}^{N_k} \vartheta_k \|K_k u\|_1 + \frac{1}{2} \|u - f_s\|_2^2 \end{cases}$$

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- $\blacktriangleright$  Interpretation: We try to find parameters  $\vartheta$  such that the minimizers of the variational model minimizes the loss function
- Closely related approaches: [Haber and Tenorio, '02], [Samuel and Tappen '09], [Peyré and Fadili '11], [De Los Reyes and Schönlieb '12], ...
- We developed semi-smooth Newton algorithms to solve the bilevel optimization problem for the optimal parameter vector  $\vartheta$ .

# Example: Image denoising





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# The Fields of Experts model

- Recall that the |x| function does not provide a very accurate match to the marginal distributions of zero-mean filters
- A much better match is obtained by the negative log student's-t distribution log(1 + |x|<sup>2</sup>/µ<sup>2</sup>) [Huang and Mumford '99].
- Let us consider the following nonconvex model [Roth, Black '09], [Samuel, Tappen '09], called the "Fields of Experts" model:

$$\mathcal{R}(u) = \sum_{k=1}^{N_{\mathcal{K}}} \sum_{i,j} \rho_k((\mathcal{K}_k u)_{i,j}),$$

where  $K_k$  are again linear operators implementing 2D convolutions with small filters  $f_k$ , that is  $f_k * u \Leftrightarrow K_k u$ , and  $\rho_k(t) = \alpha_k \log(1 + |t|^2)$ .

In contrast to the previous model, also the filters are learned.



- We again consider training data consisting of clean and noisy images (f<sub>s</sub>, g<sub>s</sub>)<sup>S</sup><sub>s=1</sub>
   We again used a bilevel optimization approach to learn the filters and functions
  - We again used a bilevel optimization approach to learn the filters and functions  $\vartheta = (f_k, \alpha_k)_{k=1}^{N_K}$

$$\begin{cases} \min_{\vartheta} L(\vartheta) = \frac{1}{2} \sum_{s=1}^{S} \|u_s(\vartheta) - g_s\|^2 + R(\vartheta) \\ \text{s.t. } u_s(\vartheta) = \arg\min_{u} \sum_{k=1}^{N_k} \sum_{i,j} \rho_k((K_k u)_{i,j}) + \frac{1}{2} \|u - f_s\|_2^2, \end{cases}$$

where  $R(\vartheta)$  is a regularization term for the learned parameters, for example one could consider the constraints

$$\mathbf{1}^T f_k = \mathbf{0}, \quad \alpha_k \ge \mathbf{0}, \quad k = 1, \dots, K$$

## Lagrangian

In order to compute gradients of the loss function with respect to ϑ, we replace the lower-level optimization problem by its first-order optimality condition (assuming s = 1 and dropping the index):

$$\sum_{k=1}^{N_{K}} K_{k}^{*} \phi_{k}(K_{k}u) + u - f = 0, \quad \phi_{k}(y) = \operatorname{diag}(\rho_{k}'(y_{1}), ..., \rho_{k}'(y_{n}),$$

where  $K_k^*$  denotes the adjoint filter and consider the Lagrangian functional

$$\mathcal{L}(u,\vartheta,\lambda) = \|u-g\|^2 + R(\vartheta) + (\sum_{k=1}^{N_K} K_k^* \phi_k(K_k u) + u - f)^T p,$$

where p is a vector of Lagrange multipliers.

► Assuming the existence of a regular local minimum in (u, v), we can invoke the classical Lagrange multiplier theorem, which guarantees the existence of multipliers p such that:

$$\begin{pmatrix} (\sum_{k=1}^{N_{\kappa}} K_{k}^{*} D\phi_{k}(K_{k}u)K_{k}+I)p+u-g \\ D_{\vartheta}R(\vartheta)+(D_{\vartheta}\sum_{k=1}^{N_{\kappa}} K_{k}^{*}\phi_{k}(K_{k}u))p \\ \sum_{k=1}^{N_{\kappa}} K_{k}^{*}\phi_{k}(K_{k}u)+u-f \end{pmatrix}=0.$$

# Implicit differentiation

For fixed  $\vartheta$ , the system can be reduced by first solving the lower level problem (last equation) for  $u^*$ , that is

$$\sum_{k=1}^{N_K} K_k^* \phi_k(K_k u^*) + u^* - f = 0,$$

then one can solve for  $p^*$  by solving the linear system

$$p^* = (\sum_{k=1}^{N_K} K_k^* D\phi_k (K_k u^*) K_k + I)^{-1} (g - u^*),$$

and finally the gradient of the loss function with respect to artheta is given by

$$\partial_{\vartheta}L(\vartheta) = D_{\vartheta}R(\vartheta) + (D_{\vartheta}\sum_{k=1}^{N_{\kappa}}K_{k}^{*}\phi_{k}(K_{k}u^{*}))(\sum_{k=1}^{N_{\kappa}}K_{k}^{*}D\phi_{k}(K_{k}u^{*})K_{k}+I)^{-1}(g-u^{*}),$$

which is nothing else then implicit differentiation.

▶ The loss function can then be minimized using any gradient-based optimization algorithm.

# The learned filters and functions

In [Chen, Ranftl, P. '14] we learned 80 filters of size 9 × 9 plus function parameters → 6480 parameters on a database of ~ 200 images using bilevel optimization

... two weeks later ...

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#### Evaluation

- Comparison with five state-of-the-art approaches: K-SVD [Elad and Aharon '06], FoE [Q. Gao and Roth '12], BM3D [Dabov et al. '07], GMM [D. Zoran et al. '12], LSSC [Mairal et al. '09]
- ▶ We report the average PSNR on 68 images of the Berkeley image data base [Chen, P. 14]

$\sigma$	KSVD	FoE	BM3D	GMM	LSSC	BL7x7	BL9x9
15	30.87	30.99	31.08	31.19	31.27	31.18	31.22
25	28.28	28.40	28.56	28.68	28.70	28.66	28.70
50	25.17	25.35	25.62	25.67	25.72	25.70	25.76

Performs as well as state-of-the-art

# Denoising results for $\sigma = 25$





# Denoising results for $\sigma = 25$





# Denoising results for $\sigma = 25$





Practical

# foe.ipynb

# Computing gradients

- Bilevel optimization is heavily time consuming since for implicit differentiation we need to:
  - Solve the lower problems exactly
  - Invert the Hessian of the lower level problem
- > Performance strongly depends on the error of the stationary point  $u^*$

# Computing gradients

- Bilevel optimization is heavily time consuming since for implicit differentiation we need to:
  - Solve the lower problems exactly
  - Invert the Hessian of the lower level problem
- ▶ Performance strongly depends on the error of the stationary point  $u^*$
- Alternative: Unroll the steps of an iterative algorithm
- The bilevel optimization problem becomes

$$\begin{cases} \min_{\vartheta} \frac{1}{2} \sum_{s=1}^{S} \left\| u_s^T(\vartheta) - g_s \right\|^2 \\ \text{s.t. } u_s^{t+1} = u_s^t - \tau^t \left( \sum_{k=1}^{N_K} K_k^* \phi_k(K_k u_s) + (u_s^t - f) \right) \\ t = 0 \dots T - 1 \end{cases}$$

- We can compute the exact gradient with respect to the model parameters using the backpropagation algorithm.
- It turns out that taking only a finite number of steps works even better....

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#### Motivation

As a motivating example, let us step back to a smooth approximation of the TV– $L^2$  (ROF) model

$$E_{\epsilon}[u, \nu] = 
u \sum_{i,j} \sqrt{|(\mathrm{D}u)_{i,j}|^2 + \epsilon^2} + rac{1}{2} ||u - g||_2^2,$$

and for various weighting parameters  $\nu$  the gradient flow with step size  $\tau$ 

$$u_{s+1} = u_s - \tau \left( \nu \mathbf{D}^* \left( \frac{\mathbf{D}u_s}{\sqrt{|(\mathbf{D}u_s)|^2 + \epsilon^2}} \right) + u_s - g \right)$$

# TV– $L^2$ classical





# TV– $L^2$ classical







# $TV-L^2$ classical





 $\mathrm{PSNR}=20.53$ 

# TV– $L^2$ classical





PSNR = 24.26

# TV– $L^2$ classical





PSNR = 26.59

# $TV-L^2$ classical





 $\mathrm{PSNR} = 19.61$ 

# TV– $L^2$ with early stopping





 $\mathrm{PSNR}=25.23$ 

# TV– $L^2$ with early stopping





 $\mathrm{PSNR}=25.55$ 

# TV– $L^2$ with early stopping





 $\mathrm{PSNR}=27.19$ 



▶ The best performance (red cross) is achieved for early stopping.

When minimizing the energy exactly the solution is "oberfitted" to the variational model and gives inferior results.
Let  $u \in \mathbb{R}^n$  be a data vector, then the variational energy is

 $\mathcal{E}[u] = \mathcal{D}[u] + \mathcal{R}[u].$ 

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Fields-of-Experts regularization:

$$\mathcal{R}[u] = \sum_{i=1}^{m} \sum_{k=1}^{N_{K}} \rho_{k}((K_{k}u)_{i})$$

with  $K_k \in \mathbb{R}^{m \times n}$  and associated nonlinear functions  $\rho_k : \mathbb{R} \to \mathbb{R}$ 

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with  $K_k \in \mathbb{R}^{m \times n}$  and associated nonlinear functions  $\rho_k : \mathbb{R} \to \mathbb{R}$  data fidelity:

$$\mathcal{D}[u] = \frac{1}{2} \|Au - b\|_2^2$$

 $A \in \mathbb{R}^{l \times n}$  and  $b \in \mathbb{R}^{l}$  fixed

Gradient flow of energy  $\mathcal{E}$  for a time  $t \in (0, T)$ :

$$\begin{split} \dot{\tilde{x}}(t) &= f(\tilde{x}(t), (K_k, \Phi_k)_{k=1}^{N_K}) = -D\mathcal{E}[\tilde{x}(t)] \\ &= -A^*(A\tilde{x}(t) - b) - \sum_{k=1}^{N_K} K_k^* \Phi_k(K_k \tilde{x}(t)), \\ &\tilde{x}(0) = x_0, \end{split}$$

with  $\tilde{x} \in C^1([0, T], \mathbb{R}^n)$ ,  $T \in \mathbb{R}^+_0$  and the functions  $\Phi_k \in \mathcal{V}^s$  are given by  $(y_1, \dots, y_m)^\top \mapsto (\rho'_k(y_1), \dots, \rho'_k(y_m))^\top$ ,

with  $\mathcal{V}^{s}$  finite dimensional subspace of  $C^{s}(\mathbb{R}^{m},\mathbb{R}^{m})$ 

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 $\min_{T \in \mathbb{R}, K_k \in \mathbb{R}^{m \times n}, \Phi_k \in \mathcal{V}^s} J(T, (K_k, \Phi_k)_{k=1}^{N_K})$ 

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cost functional:

$$J(T, (K_k, \Phi_k)_{k=1}^{N_K}) \coloneqq \frac{1}{2} \|x(1) - x_g\|_2^2$$

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constraints:

$$0 \leq T \leq T_{\max}, \quad \alpha(K_k) \leq 1, \quad \beta(\Phi_k) \leq 1, \quad K_k \mathbf{1} = \mathbf{0} \in \mathbb{R}^m,$$

 $\alpha: \mathbb{R}^{m \times n} \to \mathbb{R}_0^+$  and  $\beta: \mathcal{V}^s \to \mathbb{R}_0^+$  are continuously differentiable, coercive functions

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 $\alpha : \mathbb{R}^{m \times n} \to \mathbb{R}_0^+$  and  $\beta : \mathcal{V}^s \to \mathbb{R}_0^+$  are continuously differentiable, coercive functions transformed state equation for  $t \in (0, 1)$ :

 $\dot{x}(t) = Tf(x(t), (K_k, \Phi_k)_{k=1}^{N_K}), \qquad x(0) = x_0$ 

#### Theorem (First order necessary condition)

Let  $s \geq 1$ . For each stationary point  $(\overline{T}, (\overline{K}_k, \overline{\Phi}_k)_{k=1}^{N_K})$  of J with state  $\overline{x}$ 

$$\int_0^1 \langle \overline{
ho}(t), \dot{\overline{x}}(t) 
angle \, \mathrm{d}t = 0$$

holds true. Here,  $\overline{p} \in C^1([0,1],\mathbb{R}^n)$  denotes the adjoint state of  $\overline{x}$ , which is given as the solution to the ODE

$$\dot{\overline{p}}(t) = \sum_{k=1}^{N_{K}} \overline{K}_{k}^{*} D \overline{\Phi}_{k}(\overline{K}_{k} \overline{x}(t)) \overline{K}_{k} \overline{p}(t) + A^{*} A \overline{p}(t)$$

with terminal condition  $\overline{p}(1) = x_g - \overline{x}(1)$ .







Let  $S \ge 2$  be a fixed depth and  $\overline{\Theta} = ((\overline{K}_k, \overline{\Phi}_k)_{k=1}^{N_K})$ . State equation: Explicit forward Euler:

$$x_{s+1} = x_s + \frac{T}{S}f(x_s,\overline{\Theta})$$
  $s = 0, \dots, S-1$ 

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Explicit 2<sup>nd</sup>–order Heun:

$$x_{s+1} = x_s + \frac{T}{2S} \left( f(x_s, \overline{\Theta}) + f\left(x_s + \frac{T}{S}f(x_s, \overline{\Theta})\right) \right)$$

Let  $S \ge 2$  be a fixed depth and  $\overline{\Theta} = ((\overline{K}_k, \overline{\Phi}_k)_{k=1}^{N_K})$ . Adjoint state equation:

$$\dot{p}(t) = g(x(t), p(t), \overline{\Theta}) = \sum_{k=1}^{N_{K}} \overline{K}_{k}^{*} D\overline{\Phi}_{k}(\overline{K}_{k}x(t))\overline{K}_{k}p(t) + A^{*}Ap(t)$$

Explicit forward Euler:

$$p_{s} = p_{s+1} - \frac{T}{S}g(x_{s+1}, p_{s+1}, \overline{\Theta})$$

Explicit 2<sup>nd</sup>-order Heun:

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# Learning

For a given training set  $(x_0^i, x_g^i)_{i \in \mathcal{I}}$ , the loss for a batch  $\mathcal{B} \subset \mathcal{I}$  is given by

$$J_{\mathcal{B}}(\mathcal{T},(\mathcal{K}_k,w_k)_{k=1}^{N_K}) \coloneqq \frac{1}{2|\mathcal{B}|} \sum_{i \in \mathcal{B}} \|x_S^i - x_g^i\|_2^2$$

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subject to

$$\begin{split} & \mathcal{K}_k \in \mathcal{K} = \left\{ \mathcal{K} \in \mathbb{R}^{m \times n} : \alpha(\mathcal{K}) \leq 1, \mathcal{K}\mathbf{1} = 0 \right\}, \\ & w_k \in \mathcal{W} = \left\{ w \in \mathbb{R}^{N_w} : \beta(w) \leq 1 \right\}. \end{split}$$

Here

$$\rho'(x) = \sum_{j=1}^{N_w} w_j \psi_j(x)$$

with quadratic B–spline basis functions  $\psi_j(x) \in C^1(\mathbb{R})$ .

### Image restoration

image denoising

$$b = x_g + n$$

where

 $n \sim \mathcal{N}(0, \sigma^2 I).$ 

Default:  $\sigma = 0.1$ 

### Image restoration

#### image denoising

where

 $n \sim \mathcal{N}(0, \sigma^2 I).$ 

 $b = x_g + n$ 

Default:  $\sigma = 0.1$ 

image deblurring

$$b = A_{\tau} x_g + n$$

with blur operator  $A_{\tau}$ 

$$(x,y)\mapsto rac{1}{\sqrt{2\pi\tau^2}}\exp\left(-rac{x^2+y^2}{2\tau^2}
ight).$$

Default:  $\tau = 1.5$  and  $\sigma = 0.01$ 

## Regularization parameters - denoising



## Regularization parameters - deblurring



# Early stopping



Inference speed: 5.694ms for S = 20

# Early stopping





image denoising



image denoising

image deblurring







PSNR=20.00



PSNR=26.36

 $S = 10 \bullet T = \frac{\overline{T}}{2}$ 



PSNR=28.87



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PSNR=29.15



### Stopping time $\iff$ Noise level

Does the stopping time depend on the noise level  $\sigma$ ?

### Stopping time $\iff$ Noise level



# Stopping time $\iff$ Noise level

	$\sigma = 0.075$		$\sigma = 0.1$		$\sigma = 0.125$		$\sigma = 0.15$	
	$\overline{\mathrm{PSNR}}$	T	$\overline{\mathrm{PSNR}}$	$\overline{T}$	$\overline{\mathrm{PSNR}}$	T	$\overline{\mathrm{PSNR}}$	$\overline{T}$
full optimization of all controls optimization only of $\overline{T}$	30.05 30.00	0.724 0.757	28.72	1.082	27.72 27.73	1.445 1.514	26.95 26.95	1.433 2.055

### Stopping time $\iff$ Blur strength

Does the stopping time depend on the blur strength  $\tau$ ?

### Stopping time $\iff$ Blur strength



## Stopping time $\iff$ Blur strength

	au = 1.25		au = 1.5		au = 1.75		$\tau = 2.0$	
	$\overline{\mathrm{PSNR}}$	T	$\overline{\mathrm{PSNR}}$	$\overline{T}$	$\overline{\mathrm{PSNR}}$	T	$\overline{\mathrm{PSNR}}$	T
full optimization of all controls optimization only of $\overline{T}$	29.95 29.73	39.86 23.86	28.76	37.78	27.87 27.69	40.60 47.72	27.13 26.71	40.01 51.70
Nonlinear eigenvalue analysis of FoE regularizers

Nonlinear eigenvalue analysis of FoE regularizers Compute generalized eigenpairs  $(\lambda_j, v_j) \in \mathbb{R} \times \mathbb{R}^n$  via

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 $\rightarrow$  forward Euler scheme reduces to

$$\mathbf{v}_j - rac{T}{S} \sum_{k=1}^{N_K} \mathbf{K}_k^{ op} \mathbf{\Phi}_k(\mathbf{K}_k \mathbf{v}_j) = \left(1 - rac{\lambda_j T}{S}\right) \mathbf{v}_j,$$

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• contrast factor  $(1 - \frac{\lambda_i T}{S})$  determines global contrast change

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• contrast factor  $(1 - \frac{\lambda_j T}{S})$  determines global contrast change

- holds only for one step
- eigenvalue determines contrast preservation

#### Estimation of generalized eigenpairs

Compute  $N_v$  generalized eigenpairs by solving

$$\min_{\{\mathbf{v}_j\}_{j=1}^{N_{\mathbf{v}}}}\sum_{j=1}^{N_{\mathbf{v}}}\left\|\sum_{k=1}^{N_{\mathbf{K}}}K_k^{\top}\Phi_k(K_k\mathbf{v}_j)-\Lambda(\mathbf{v}_j)\mathbf{v}_j\right\|_2^2,$$

where

$$\Lambda(v) = \frac{\left\langle \sum_{k=1}^{N_{K}} K_{k}^{\top} \Phi_{k}(K_{k}v), v \right\rangle}{\|v\|_{2}^{2}}$$

is generalized Rayleigh quotient.

#### Estimation of generalized eigenpairs

Compute  $N_v$  generalized eigenpairs by solving

$$\min_{\{\mathbf{v}_j\}_{j=1}^{N_{\mathbf{v}}}} \sum_{j=1}^{N_{\mathbf{v}}} \left\| \sum_{k=1}^{N_{\mathbf{K}}} K_k^\top \Phi_k(K_k v_j) - \Lambda(v_j) v_j \right\|_2^2,$$

where

$$\Lambda(\mathbf{v}) = \frac{\left\langle \sum_{k=1}^{N_{K}} K_{k}^{\top} \Phi_{k}(K_{k}\mathbf{v}), \mathbf{v} \right\rangle}{\|\mathbf{v}\|_{2}^{2}}$$

is generalized Rayleigh quotient.

Optimization by accelerated gradient method with backtracking.

### Nonlinear eigenpairs for image denoising



### Nonlinear eigenpairs for image deblurring



#### Overview

Parameter learning in variational models

The Fields of Experts model

Early stopping

Total Deep Variation

Learning with graphical models

#### Variational Formulation of Linear Inverse Problems

▶  $x \in \mathbb{R}^{nC}$  restored image (size  $n = n_1 \cdot n_2$ , *C* channels)

$$x \in \operatorname*{argmin}_{\widehat{x} \in \mathbb{R}^{n^{C}}} \left\{ \mathcal{E}(\widehat{x}, \theta, z) \coloneqq \mathcal{D}(\widehat{x}, z) + \mathcal{R}(\widehat{x}, \theta) \right\}$$

- ► data fidelity term  $\mathcal{D}(x, z) = \frac{1}{2} ||Ax z||_2^2$  for fixed task-dependent  $A \in \mathbb{R}^{IC \times nC}$  and observed data  $z \in \mathbb{R}^{IC}$
- ► total deep variation: parametric deep multi-scale regularizer *R* depending on learned training parameters θ ∈ Θ ⊂ ℝ<sup>p</sup>

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► data fidelity term  $\mathcal{D}(x, z) = \frac{1}{2} ||Ax - z||_2^2$  for fixed task-dependent  $A \in \mathbb{R}^{IC \times nC}$  and observed data  $z \in \mathbb{R}^{IC}$ 

► total deep variation: parametric deep multi-scale regularizer *R* depending on learned training parameters θ ∈ Θ ⊂ ℝ<sup>p</sup>

Gradient flow for  $t \in (0, T)$ :  $\dot{\tilde{x}}(t) = f(\tilde{x}(t), \theta, z) := -A^{\top}(A\tilde{x}(t) - z) - \nabla_1 \mathcal{R}(\tilde{x}(t), \theta),$  $\tilde{x}(0) = x_{\text{init}}$ 

Reparametrization  $x(t) = \tilde{x}(tT)$  results in equivalent gradient flow for  $t \in (0, 1)$ :  $\dot{x}(t) = Tf(x(t), \theta, z), \qquad x(0) = x_{init}$ 

#### Total Deep Variation



$$\begin{split} & \mathcal{K} \in \mathbb{R}^{nm \times nC} \text{ learned} \\ & \text{convolution kernel} \\ & (\sum_{i=1}^{nC} \mathcal{K}_{j,i} = 0 \text{ for } j = 1, \dots, nm), \end{split}$$

 $f: \mathbb{R}^{nm} \to \mathbb{R}^{nq}$  multiscale convolutional neural network,

 $w \in \mathbb{R}^q$  learned weight vector,

 $\begin{aligned} \theta &= (K, K'_{s,t}, w) \text{ for } l \in \{1, 2, 3\}, \\ s &\in \{1, \dots, 5\}, \ t \in \{1, 2\}, \end{aligned}$ 

 $r(x,\theta) \coloneqq w^{\top} f(Kx),$ 

Training set:  $N \in \mathbb{N}$  triples  $(x_{init}^i, y^i, z^i)_{i=1}^N$  $\succ x_{init}^i \in \mathbb{R}^{nC}$  initial image $\flat y^i \in \mathbb{R}^{nC}$  ground truth image $\flat z^i \in \mathbb{R}^{lC}$  observed data

noise  $n^i \sim \mathcal{N}(0, \sigma^2) \Rightarrow x^i_{\text{init}} = z^i = y^i + n^i$ 

Training set:  $N \in \mathbb{N}$  triples  $(x_{init}^i, y^i, z^i)_{i=1}^N$   $x_{init}^i \in \mathbb{R}^{nC}$  initial image  $y^i \in \mathbb{R}^{nC}$  ground truth image  $z^i \in \mathbb{R}^{lC}$  observed data Example (additive Gaussian image denoising): A = I, ground truth  $y^i$  corrupted by

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►  $x_{init}^i \in \mathbb{R}^{nC}$  initial image

- ▶  $y^i \in \mathbb{R}^{nC}$  ground truth image
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Example (additive Gaussian image denoising): A = I, ground truth  $y^i$  corrupted by noise  $n^i \sim \mathcal{N}(0, \sigma^2) \Rightarrow x_{init}^i = z^i = y^i + n^i$ 

Sampled optimal control problem with convex and coercive loss /:

$$\inf_{T \in [0, T_{\max}], \theta \in \Theta} \left\{ J(T, \theta) \coloneqq \frac{1}{N} \sum_{i=1}^{N} I(x^{i}(1) - y^{i}) \right\}$$

s.t. state equation for each sample  $(i = 1, ..., N \text{ and } t \in (0, 1))$ 

 $\dot{x}^i(t) = Tf(x^i(t), \theta, z^i), \qquad x^i(0) = x^i_{\mathrm{init}}$ 

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#### Theorem

The minimum in the sampled optimal control problem is attained.

Discretized Optimal Control Problem

$$\inf_{T \in [0, T_{\max}], \theta \in \Theta} \left\{ J_{S}(T, \theta) \coloneqq \frac{1}{N} \sum_{i=1}^{N} I(x_{S}^{i} - y^{i}) \right\}$$

subject to discrete state equation (s = 0, ..., S - 1 and i = 1, ..., N)

$$\begin{aligned} x_{s+1}^{i} &= x_{s}^{i} - \frac{T}{S} A^{\top} (A x_{s+1}^{i} - z^{i}) - \frac{T}{S} \nabla_{1} \mathcal{R}(x_{s}^{i}, \theta), \\ x_{0}^{i} &= x_{\text{init}}^{i} \in \mathbb{R}^{nC} \end{aligned}$$

depth  $S \in \mathbb{N}$  a priori fixed

Discretized Optimal Control Problem

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depth  $S \in \mathbb{N}$  a priori fixed Equivalent state equation:  $x_{s+1}^i = \tilde{f}(x_s^i, T, \theta, z^i)$  with

$$\widetilde{f}(x, T, \theta, z) \coloneqq (I + \frac{T}{S}A^{\top}A)^{-1}(x + \frac{T}{S}(A^{\top}z - \nabla_1\mathcal{R}(x, \theta)))$$

Let  $(\overline{T}, \overline{\theta})$  be a pair of optimal control parameters with the corresponding state  $\{\overline{x}_s^i\}_{s=0,...,S}^{i=1,...,N}$ . We define the Hamiltonian

$$H: \mathbb{R}^{nC} \times \mathbb{R}^{nC} \times [0, T_{\max}] \times \Theta \times \mathbb{R}^{lC} \to \mathbb{R}$$
$$(x, p, T, \theta, z) \mapsto \langle p, \widetilde{f}(x, T, \theta, z) \rangle.$$

If  $\nabla \tilde{f}(\bar{x}_s^i, \overline{T}, \bar{\theta}, z^i)$  has full rank for all i = 1, ..., N and s = 0, ..., S, then there exists an adjoint process  $\{\bar{p}_s^i\}_{s=0,...,S}^{i=1,...,N}$  s.t.

$$\begin{split} \overline{x}_{s+1}^{i} &= \nabla_{2} H(\overline{x}_{s}^{i}, \overline{p}_{s+1}^{i}, \overline{T}, \overline{\theta}, z^{i}), \qquad \qquad \overline{x}_{0}^{i} = x_{\text{init}}^{i}, \\ \overline{p}_{s}^{i} &= \nabla_{1} H(\overline{x}_{s}^{i}, \overline{p}_{s+1}^{i}, \overline{T}, \overline{\theta}, z^{i}), \qquad \qquad \overline{p}_{S}^{i} = -\frac{1}{N} \nabla I(\overline{x}_{S}^{i} - y^{i}). \end{split}$$

Finally, the solution is optimal in the sense that

$$\sum_{i=1}^{N} H(\overline{x}_{s}^{i}, \overline{p}_{s+1}^{i}, \overline{T}, \overline{\theta}, z^{i}) \geq \sum_{i=1}^{N} H(\overline{x}_{s}^{i}, \overline{p}_{s+1}^{i}, T, \theta, z^{i})$$

for all  $T \in [0, T_{\max}]$  and  $\theta \in \Theta$ .

discrete adjoint states  $p_s^i$  computed via discrete Pontryagin maximum principle:

$$\begin{aligned} \overline{p}_{s}^{i} &= \nabla_{1} H(\overline{x}_{s}^{i}, \overline{p}_{s+1}^{i}, \overline{T}, \overline{\theta}, z^{i}) \\ &= (I - \frac{\overline{T}}{\overline{S}} \nabla_{1}^{2} \mathcal{R}(\overline{x}_{s}^{i}, \overline{\theta}))(I + \frac{\overline{T}}{\overline{S}} A^{\top} A)^{-1} \overline{p}_{s+1}^{i}, \\ \overline{p}_{S}^{i} &= -\frac{1}{N} \nabla I(\overline{x}_{S}^{i} - y^{i}). \end{aligned}$$

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#### Theorem (Optimality condition)

Let  $(\overline{T}, \overline{\theta})$  be a stationary point of  $J_S$  with associated states  $\overline{x}_s^i$  and adjoint states  $\overline{p}_s^i$ . We further assume that  $\nabla \tilde{f}(\overline{x}_s^i, \overline{T}, \overline{\theta}, z^i)$  has full rank for all i = 1, ..., N and s = 0, ..., S. Then, we have

$$-\frac{1}{N}\sum_{s=0}^{S-1}\sum_{i=1}^{N}\langle \overline{p}_{s+1}^{i}, (I+\frac{\overline{T}}{5}A^{T}A)^{-1}(\overline{x}_{s+1}^{i}-\overline{x}_{s}^{i})\rangle = 0.$$





ground truth image





 $\mathrm{PSNR}=20.18$ 





 $\mathrm{PSNR}=24.33$ 





 $\mathrm{PSNR}=26.61$ 





 $\mathrm{PSNR}=29.63$ 





PSNR = 32.91





PSNR = 33.92





PSNR = 33.04





 $\mathrm{PSNR} = 32.34$ 

### Numerical Results (Gaussian Image Denoising)





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### Numerical Results (Gaussian Image Denoising)



 $S \mapsto \frac{1}{N} \sum_{i=1}^{N} \text{PSNR}(x_S^i, y^i)$ 

Top:  $S \mapsto \frac{1}{N} \sum_{i=1}^{N} \operatorname{PSNR}(x_{S}^{i}, y^{i})$ 

Bottom:  $S \mapsto \overline{T}$ 

#### Numerical Results (Gaussian Image Denoising)

 $T \mapsto \mathrm{PSNR}(x_S^i, y^i)$ 







Top:  $T \mapsto \text{PSNR}(x_S^i, y^i)$ 

Bottom:  $T \mapsto -\sum_{s=0}^{S} \langle p_{s+1}^{i}, x_{s+1}^{i} - x_{s}^{i} \rangle$ 

Averages across samples are depicted by red curves
# Numerical Results (Gaussian Image Denoising)

Data set	$\sigma$	BM3D	TNRD	DnCNN	FFDNet	N <sup>3</sup> Net	FOCNet	TDV <sup>3</sup>
Set12	15	32.37	32.50	32.86	32.75	-	33.07	33.01
	25	29.97	30.05	30.44	30.43	30.55	30.73	30.66
	50	26.72	26.82	27.18	27.32	27.43	27.68	27.59
BSDS68	15	31.08	31.42	31.73	31.63	-	31.83	31.82
	25	28.57	28.92	29.23	29.19	29.30	29.38	29.37
	50	25.60	25.97	26.23	26.29	26.39	26.50	26.45
Urban100	15	32.34	31.98	32.67	32.43	-	33.15	32.87
	25	29.70	29.29	29.97	29.92	30.19	30.64	30.38
	50	25.94	25.71	26.28	26.52	26.82	27.40	27.04
# Parameters			26,645	555,200	484,800	705,895	53,513,120	427,330

TDV<sup>3</sup> slightly worse than FOCNet (state-of-the-art), but

- FOCNet only applicable for denoising,
- ► TDV<sup>3</sup> has less than 1 % of the parameters of FOCNet,
- ▶ rigorous mathematical theory for TDV<sup>3</sup> available

# Understanding TDV

Nonlinear eigenmode analysis for TDV<sup>3</sup>:

 $\overline{x} \in \operatorname*{argmin}_{x} \mathcal{R}(x, \theta) \quad \text{s.t.} \ \|x\|_2 = \|x_{\mathrm{init}}\|_2$ 



# ${\sf Understanding} \ {\sf TDV}$

Nonlinear eigenmode analysis for TDV<sup>3</sup>:

 $\overline{x} \in \operatorname*{argmin}_{x} \mathcal{R}(x, \theta) \quad \text{s.t.} \ \|x\|_2 = \|x_{\mathrm{init}}\|_2$ 



## Sensitivity Analysis (Gaussian Image Denoising)

- (T, θ), (T, θ) two pairs of control parameters (obtained from two different training datasets)
- ► x, x̃ ∈ (ℝ<sup>nC</sup>)<sup>(S+1)</sup> two solutions of state equation with same observed data z and initial condition x<sub>init</sub>, i.e.

$$x_{s+1} = \widetilde{f}(x_s, T, \theta, z), \quad \widetilde{x}_{s+1} = \widetilde{f}(\widetilde{x}_s, \widehat{T}, \widehat{\theta}, z)$$

for  $s = 1, \ldots, S - 1$  and  $x_0 = \widetilde{x}_0 = x_{\text{init}}$ 

upper bound estimate by ODE theory



- ▶ single image super-resolution with scale factor  $\gamma \in \{2, 3, 4\}$
- ▶ full resolution ground truth image  $y^i \in \mathbb{R}^{nC}$
- linear downsampling operator A as implementation of scale factor-dependent interpolation convolution kernel in conjunction with stride
- ► observed low resolution image  $z^i = Ay^i \in \mathbb{R}^{nC/\gamma^2}$





ground truth image



noisy



TDV



TDV (continued)

Data set	Scale	MemNet	VDSR	DRRN	OISR-LF-s	TDV <sup>3</sup>
Set14	×2 ×3 ×4	33.28 30.00 28.26	33.03 29.77 28.01	33.23 29.96 28.21	33.62 30.35 28.63	33.35 29.96 28.41
BSDS100	$\begin{array}{c} \times 2 \\ \times 3 \\ \times 4 \end{array}$	32.08 28.96 27.40	31.90 28.82 27.29	32.05 28.95 27.38	32.20 29.11 27.60	32.18 28.98 27.50
# Parameters		585,435	665,984	297,000	1,370,000	428,970

# Transfering TDV to medical imaging

2D CT reconstruction for angular undersampling



PSNR = 43.51

PSNR = 35.03

PSNR = 27.75

#### undersampled MRI reconstruction



4-fold undersampling PSNR = 24.98

our result PSNR = 48.29

reference image

our result PSNR = 38.55



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### Learning with graphical models

- Finally, we consider learning parameters with graphical models for image labeling.
- For many years, both the unary terms and binary terms have been computed based on handcrafted functions.
- Cannot compete with recent deep-learning methods.
- ► We propose to ...

### Learning with graphical models

- Finally, we consider learning parameters with graphical models for image labeling.
- For many years, both the unary terms and binary terms have been computed based on handcrafted functions.
- Cannot compete with recent deep-learning methods.
- ► We propose to ...
- (i) Learn neural networks that compute  $\theta = (\theta_i, \theta_{i,j})$  from the input.
- (ii) Adopt the graphical model as an inference layer in the network.

• Given a stereo image pair, compute the disparity (inverse depth)



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 $\theta_i(x_i)$ 

Given a stereo image pair, compute the disparity (inverse depth)



 $\theta_i(x_i)$ 

 $\theta_{i,j}(x_i, x_j)$ 

Given a stereo image pair, compute the disparity (inverse depth)



$$\sum_{i\in\mathcal{V}} \theta_i(x_i) + \sum_{(i,j)\in\mathcal{E}} \theta_{i,j}(x_i,x_j)$$

Given a stereo image pair, compute the disparity (inverse depth)



$$\min_{x \in \mathcal{L}} E(x, \theta) := \sum_{i \in \mathcal{V}} \theta_i(x_i) + \sum_{(i,j) \in \mathcal{E}} \theta_{i,j}(x_i, x_j)$$

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Two main issues:

- (i) Efficient solution of the inference layer
- (ii) End-to-end learning

### Learning

For learning the parameters ϑ of the neural network, we consider a loss function ℓ that compares the output of the image labeling problem x(ϑ) with the ground truth labels x<sup>†</sup>, e.g.

$$\ell(x(\vartheta), x^{\dagger}) = \left\| x(\vartheta) - x^{\dagger} \right\|_{1}$$

▶ The learning problem represents a bilevel optimization problem:

 $\min_{\vartheta} \ell(x(\vartheta), g), \quad \text{s.t. } x(\vartheta) \in \arg\min_{x \in \mathcal{L}} \in E(x, f(\vartheta)),$ 

- Hard to solve, because  $x(\vartheta)$  does not continuously depend on  $\vartheta$ .
- We approximate the problem by constructing a differentiable upper bound similar to the structured output SVM [Tsochantaridis et al. '04]

▶ We use the following chain of upper bounds:

$$\max_{x \in \arg\min_{x \in \mathcal{L}} E(x,f)} \ell(x,x^{\dagger}) \leq \max_{x \in \mathcal{L}: E(x,f) \leq E(x^{\dagger},f)} \ell(x,x^{\dagger})$$

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$$\leq \max_{x \in \mathcal{L}: E(x,f) \leq E(x^{\dagger},f)} \ell(x,x^{\dagger}) + E(x^{\dagger},f) - E(x,f)$$

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$$\leq \max_{x \in \mathcal{L}} \ell(x,x^{\dagger}) + E(x^{\dagger},f) - E(x,f)$$
$$= \psi(\hat{x},x^{\dagger},f)$$

where  $\hat{x} = \arg \max_{x \in \mathcal{L}} \ell(x, x^{\dagger}) - E(x, f).$ 

The function ψ is linear in f (in the lifted space), hence it is a maximum over linear functions → convex.

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where  $\hat{x} = \arg \max_{x \in \mathcal{L}} \ell(x, x^{\dagger}) - E(x, f)$ .

- The function ψ is linear in f (in the lifted space), hence it is a maximum over linear functions → convex.
- Computing the upper bound requires to solve the labeling problem but with loss-augmented unary terms.
- The resulting surrogate function is differentiable with respect to the unaries  $f_i$

 $D_{f_i}\psi(\hat{x},x^{\dagger},f)=\delta(x_i^{\dagger})-\delta(\hat{x}_i)$   $\rightsquigarrow$ 

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- ► The function \u03c6 is linear in f (in the lifted space), hence it is a maximum over linear functions \u2223 convex.
- Computing the upper bound requires to solve the labeling problem but with loss-augmented unary terms.
- The resulting surrogate function is differentiable with respect to the unaries  $f_i$

$$D_{f_i}\psi(\hat{x},x^{\dagger},f) = \delta(x_i^{\dagger}) - \delta(\hat{x}_i) \quad \rightsquigarrow \underbrace{D_{f_i}\psi(\hat{y},y^{\dagger},f) = y_i^{\dagger} - \hat{y}_i}_{\text{in the lifted space}}$$

▶ We use the following chain of upper bounds:

$$\max_{x \in \arg\min_{x \in \mathcal{L}} E(x,f)} \ell(x,x^{\dagger}) \leq \max_{x \in \mathcal{L}: E(x,f) \leq E(x^{\dagger},f)} \ell(x,x^{\dagger})$$
$$\leq \max_{x \in \mathcal{L}: E(x,f) \leq E(x^{\dagger},f)} \ell(x,x^{\dagger}) + E(x^{\dagger},f) - E(x,f)$$
$$\leq \max_{x \in \mathcal{L}} \ell(x,x^{\dagger}) + E(x^{\dagger},f) - E(x,f)$$
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where  $\hat{x} = \arg \max_{x \in \mathcal{L}} \ell(x, x^{\dagger}) - E(x, f)$ .

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 $\rightarrow$ 

- Computing the upper bound requires to solve the labeling problem but with loss-augmented unary terms.
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$$\mathcal{D}_{f_i}\psi(\hat{x},x^{\dagger},f) = \delta(x_i^{\dagger}) - \delta(\hat{x}_i)$$

$$\underbrace{D_{f_i}\psi(\hat{y}, y^{\dagger}, f) = y_i^{\dagger} - \hat{y}_i}_{\text{in the lifted space}}$$

Similar formula for the binary weights  $f_{i,j}$ .



 $D_{f_i}\psi(\hat{x},x^{\dagger},f) = \delta(x_i^{\dagger}) - \delta(\hat{x}_i)$ 

--- Loss margin

 $\sim \rightarrow$ 

# Graphical Explanation



 $D_{f_i}\psi(\hat{x},x^{\dagger},f) = \delta(x_i^{\dagger}) - \delta(\hat{x}_i)$ 

--- Loss margin

 $\rightarrow$ 



# Training

#### Data bases

- Middlebury Stereo Version 3
- KITTI 2015

#### Training

- Learning is performed using stochastic subgradient descent with momentum
- First, we perform a CNN-only pre-training, followed by a joint training



Benchmark	Method	CNN	+CRF	+Joint	+PW
Middlebury	CNN3	23.89	11.18	9.48	9.45
winduiedui y	CNN7	18.58	9.35	8.05	7.88
	CNN3	28.38	6.33	6.11	4.75
V;++; 2015	CNN7	13.08	4.79	4.60	4.04
Kitti 2013	[28]	5.99	4.31	-	-
	[55]	13.56	4.45	-	-

#### Experiments - Middlebury Stereo



#### Experiments - Middlebury Stereo



# Experiments - Kitti 2015



# Experiments - Kitti 2015


## Kitti 2015 - Quality of groundtruth



ContentCNN

## Extension to motion estimation (Sintel)