Level-set MCMC
Curve Sampling

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Outline

1. Overview
2. Curve evolution
3. Markov chain Monte Carlo
4. Curve sampling
5. Examples
6. Conditional simulation
Overview

- Curve evolution attempts to find a curve $C$ (or curves $C_i$) that best segment an image (according to some model).
- Goal is to minimize an energy functional $E(C)$ (view as a negative log likelihood).
- Find a local minimum using gradient descent.
Sampling instead of optimization

• Draw multiple samples from a probability distribution $p$ (e.g., uniform, Gaussian)

• Advantages:
  - Naturally handles multi-modal distributions
  - Can get out of local minima
  - Higher-order statistics (e.g., variances)
  - Conditional simulation
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Planar curves

• A curve is a function $\vec{C} : [0, 1] \rightarrow \mathbb{R}^2$

• We wish to minimize an energy functional with a data fidelity term and regularization term:

$$E(\vec{C}) = D(y|\vec{C}) + R(\vec{C})$$

• This results in a gradient flow:

$$\frac{d\vec{C}}{dt}(p) = \vec{F}(p)$$

• We can write any flow in terms of the normal:

$$\frac{d\vec{C}}{dt}(p) = f(p)\vec{N}(p)$$
Level-Set Methods

• A curve is a function (infinite dimensional)

• A natural implementation approach is to use marker points on the boundary (snakes)
  ▪ Reinitialization issues
  ▪ Difficulty handling topological change

• Level set methods instead evolve a surface (one dimension higher than our curve) whose zeroth level set is the curve (Sethian and Osher)
Embedding the curve

- Force level set $\Psi$ to be zero on the curve
  $$\Psi(\vec{C}(p)) = 0$$
  $$\forall p \in [0, 1]$$
- Chain rule gives us
  $$\frac{d\Psi}{dt} = -\frac{d\vec{C}}{dt} \cdot \nabla \Psi$$
  $$= -f||\nabla \Psi||$$
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General MAP Model

\[ p(x|y; S) \propto p(y|x; S)p(x; S) \]

- For segmentation:
  - \( x \) is a curve
  - \( y \) is the observed image (can be vector)
  - \( S \) is a shape model
  - Data model usually IID given the curve
- We wish to sample from \( p(x|y; S) \), but cannot do so directly
Markov Chain Monte Carlo

- Class of sampling methods that iteratively generate candidates based on a previous iterate (forming a Markov chain)
- Instead of sampling from $p(x|y;S)$, sample from a proposal distribution $q$ and keep samples according to an acceptance rule $a$
- Examples include Gibbs sampling, Metropolis-Hastings
Metropolis-Hastings

- Metropolis-Hastings algorithm:
  1. Start with $x^0$
  2. At time $t$, generate candidate $\phi^t$ (given $x^{t-1}$)
  3. Calculate Hastings ratio:
     \[ r^t = \frac{p(\phi^t)}{p(x^{t-1})} \cdot \frac{q(x^{t-1}|\phi^t)}{q(\phi^t|x^{t-1})} \]
  4. Set $x^t = \phi^t$ with probability $\min(1, r^t)$, otherwise $x^t = x^{t-1}$
  5. Go back to 2
Asymptotic Convergence

- We want to form a Markov chain such that its stationary distribution is $p(x)$:
  \[ p(x) = \int p(\phi) T(x|\phi) d\phi \]

- To guarantee asymptotic convergence, sufficient conditions are:
  1) Ergodicity
  2) Detailed balance
  \[ p(x^{t-1}) q(\phi^t|x^{t-1}) a(\phi^t|x^{t-1}) = p(\phi^t) q(x^{t-1}|\phi^t) a(x^{t-1}|\phi^t) \]
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MCMC Curve Sampling

• Generate perturbation on the curve:

\[ \tilde{C}'(s) = \tilde{C}(s) + f(s)\tilde{N}(s)dt \]

• Sample by adding smooth random fields:

\[ f \sim N(0, \Sigma) \]

• \( \Sigma \) controls the degree of smoothness in field

• Note for portions where \( f \) is negative, shocks may develop (so called prairie fire model)

• Implement using white noise and circular convolution
Smoothness issues

- While detailed balance assures asymptotic convergence, may need to wait a very long time
- In this case, smooth curves have non-zero probability under $q$, but are very unlikely to occur
- Can view accumulation of perturbations as
  \[ F(s) = \sum_i f_i(s) = h \ast \sum_i n_i \]
  (h is the smoothing kernel, $n_i$ is white noise)
- Solution: make $q$ more likely to move towards high-probability regions of $p$
Adding mean force

- We can add deterministic elements to $f$ (i.e., a mean to $q$):
  $$f \sim N(-\kappa + \gamma, \Sigma)$$
  $$f(s) = \beta r(s) - \alpha \kappa(s) + \gamma$$

- The average behavior should then be to move towards higher-probability areas of $p$

- In the limit, setting $f$ to be the gradient flow of the energy functional results in always accepting the perturbation
Coverage/Detailed balance

- It is easy to show we can go from any curve $C_1$ to any other curve $C_2$ (shrink to a point)

- For detailed balance, we need to compute probability of generating $C'$ from $C$ (and vice versa)

\[
\tilde{C}'(s) = \tilde{C}(s) + f(s)\tilde{N}(s)dt
\]
\[
\tilde{C}(s) = \tilde{C}'(s) + f'(s)\tilde{N}'(s)dt
\]

- Probability of going from $C$ to $C'$ is the probability of generating $f$ (which is Gaussian) and the reverse is the probability of $f'$ (also Gaussian)
Approximations to $q$

- Relationship between $f$ and $f'$ complicated due to the fact that the normal function changes

- $f'$ does not always exist (given an $f$). Unknown what conditions on $f$ are necessary to guarantee existence.

- Various levels of exactness
  - Assume $\tilde{N} = \tilde{N'}$ (then $f' = -f$)
  - Infinitesimal approximation (ignore tangential):
    \[ f'(s) = < -f(s)\tilde{N}(s), \tilde{N}'(s) > \]
  - Trace along $\tilde{N}$ (technical issues)

- Unknown how approximations affect convergence
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SAD Target

• We define symmetric area difference (SAD) as:

$$d_{SAD}(\psi_1, \psi_2) = \int_{\Omega} (\mathcal{H}(-\psi_1(x)) - \mathcal{H}(-\psi_2(x)))^2 \, dx$$

• Use a Boltzmann distribution:

$$p(\tilde{C}|\tilde{C}_0) = \frac{1}{Z} \exp\left(-\frac{d_{SAD}(\tilde{C}, \tilde{C}_0)}{T}\right)p(\tilde{C})$$

• T is a parameter we can use to control how likely we are to keep less likely samples

• We will keep a sample with T log(2) additional errors with probability ½

• Single mode distribution
Target Shape
Initialization
Most likely samples
Least likely samples
“Confidence intervals”
Doubling the temperature
Synthetic noisy image

- Piecewise-constant observation model:
  \[ y(x) = \mu(x) + n(x) \]
- Chan-Vese energy functional:
  \[ E(\mathcal{C}) = \int \int_{R_0} (y - \mu_0)^2 dx + \int \int_{R_1} (y - \mu_1)^2 dx + \alpha \oint_{\mathcal{C}} ds \]
- Probability distribution (T=2\sigma^2):
  \[ p(\mathcal{C}) = \frac{1}{Z} \exp(-E(\mathcal{C})/T) \]
Prostate in a Haystack
Most likely samples
Least likely samples
Confidence intervals
When “best” is not best

- In this example, the most likely samples under the model are not the most accurate according to the underlying truth.

- 10%/90% “confidence” bands do a good job of enclosing the true answer.

- Histogram image tells us more uncertainty in upper-right corner.

- “Median” curve is quite close to the true curve.

- Optimization would result in subpar results.
Bias-corrected prostate

• “Expert” segmentation, add noise (simulate body coil image)
Learn probability densities

- Use histograms
- Learn pdf inside $p(y|1)$ and pdf outside $p(y|0)$ and assume iid given curve:

$$E(\hat{C}) = -\int_{\Omega} \log p(y(x)|\mathcal{H}(\Psi(x))) \, dx + \alpha \int_{\hat{C}} ds$$
Most likely samples
Least likely samples
Confidence intervals
Confidence intervals (with histogram)
Multimodality and convergence

- Natural multimodal distribution
- Burn-in time is not long enough (otherwise more samples would have clustered near the more-likely mode)
- When starting near one mode, need a lot of time to traverse valley between modes
- Clustering could help with presenting results
Gravity inversion

• Supplement to standard seismic data to segment bottom salt using an array of surface gravimeters (~$10^{-15}$ N accuracy)

• Subtract base effects (geoid, centrifugal force, etc.) to leave salt effects:

$$\tilde{g}(i) = G \int_{\Omega} \frac{\rho(x; \vec{C}) \hat{r}_i(x)}{\| \hat{r}_i(x) \|^2} \, dx$$

• Assume constant density inside and outside:

$$\rho(x; \vec{C}) = \Delta \rho \mathcal{H}(-\Psi(x))$$

• Model energy as L2 estimation error (probability as Boltzmann distribution):

$$E(\vec{C}) = \sum_{i=1}^{N_{\text{array}}} \| \tilde{g}_{\text{obs}}(i) - \tilde{g}(i; \vec{C}) \|^2 + \alpha \int_{\vec{C}} ds$$
A strange segmentation problem

X- and z-components of gravity profile for synthetic salt body
Circle salt
Most likely samples
Least likely samples
Confidence intervals
Notable features

• Measurement points << image pixels, but we can do a reasonable job

• Much higher uncertainty at the bottom than the top (weaker measurements)

• Less uncertainty in middle than on sides

• Median of histogram not necessarily related to median of distribution
Mystery example

- Same x- and z-components of gravity
- Synthetic image with unknown truth
Initial state
Most likely samples
Least likely samples
Confidence intervals
Gravity error

![Graphs showing gravity error over x-component and z-component]
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User Information

- In many problems, the model admits many reasonable solutions
- Currently user input largely limited to initialization
- We can use user information to reduce the number of reasonable solutions
  - Regions of inclusion or exclusion
  - Partial segmentations
- Can help with both convergence speed and accuracy
- Interactive segmentation
Conditional simulation

- With conditional simulation, we are given the values on a subset of the variables
- We then wish to generate sample paths that fill in the remainder of the variables (e.g., simulating Brownian motion)
Simulating curves

• Say we are given $C_s$, a subset of $C$ (with some uncertainty associated with it)

• We wish to sample the unknown part of the curve $C_u$

• One way to view is as sampling from:

$$p(y|\tilde{C})p(\tilde{C}) = p(y|\tilde{C})p(\tilde{C}_u|\tilde{C}_s)p(\tilde{C}_s)$$

• Difficulty is being able to evaluate the middle term as theoretically need to integrate $p(C)$
Simplifying Cases

Under special cases, evaluation of \( p(\vec{C}_u | \vec{C}_s) \) is tractable:

1. When \( C \) is low-dimensional (can do analytical integration or Monte-Carlo integration)
2. When \( C_s \) is assumed to be exact
3. When \( p(C) \) has special form (e.g., independent)
4. When willing to approximate
Chan-Vese in 3D

- Energy functional with surface area regularization:
  \[ E(\vec{C}) = \frac{1}{2\sigma_1^2} \iint_R (y - \mu_1)^2 \, dx + \frac{1}{2\sigma_2^2} \iint_R (y - \mu_2)^2 \, dx \]
  \[ + \alpha \oint_{\vec{C}} \, dA \]

- With a slice-based model, we can write the regularization term as:
  \[ \oint_{\vec{C}} \, dA = \sum_{i=1}^{n-1} \iint_{\vec{c}_i \oplus \vec{c}_{i+1}} \, dA \]

where \( \vec{c}_i \oplus \vec{c}_{i+1} \) is the surface between \( c_i \) and \( c_{i+1} \)
Zero-order hold approximation

• Approximate volume as piecewise-constant “cylinders”:
  \[ \vec{C}(s, z) = \vec{c}_i(s), \ \forall \ |z - i\Delta z| < \frac{\Delta z}{2} \]

• Then we see that the surface areas are:
  \[
  \int \int \int dA = \frac{\Delta z}{2} \int ds + \frac{\Delta z}{2} \int ds + \int \int dx
  \]

• We see terms related to the curve length and the difference between neighboring slices

• Upper bound to correct surface area
Overall regularization term

• Adding everything together results in:

\[ \oint_C dA = \nabla z \sum_{i=1}^{n} \oint_{C_i} ds + \sum_{i=1}^{n-1} \int \int_{R_{i,i+1}^{\text{diff}}} dx \]

self potentials

edge potentials
2.5D Approach

• In 3D world, natural (or built-in) partition of volumes into slices

• Assume Markov relationship among slices

• Then have local potentials (e.g., PCA) and edge potentials (coupling between slices)

• Naturally lends itself to local Metropolis-Hastings approach (iterating over the slices)
2.5D Model

- We can model this as a simple chain structure with pairwise interactions
- This admits the following factorization:

\[
p(Y|\vec{C}) = \prod_{i=1}^{n} p(y_i|\vec{c}_i)
\]

\[
p(\vec{C}) = \prod_{i=1}^{n} \psi_i(\vec{c}_i) \prod_{i=1}^{n-1} \psi_{i,i+1}(\vec{c}_i, \vec{c}_{i+1})
\]
Partial segmentations

• Assume that we are given segmentations of every other slice

• We now want to sample surfaces conditioned on the fact that certain slices are fixed

• Markovianity tells us that \( c_2 \) and \( c_4 \) are independent conditioned on \( c_3 \)
Log probability for $c_2$

- We can then construct the probability for $c_2$ conditioned on its neighbors using the potential functions defined previously:

$$\ell(\vec{c}_2 | y_2, \vec{c}_1, \vec{c}_3) = \ell(y_2 | \vec{c}_2) + \alpha [\Delta z \int_{\vec{c}_2} ds + d_{\text{SAD}}(\vec{c}_2, \vec{c}_1) + d_{\text{SAD}}(\vec{c}_2, \vec{c}_3)]$$
Results

Neighbor segmentations

Our result (cyan) with expert (green)
Larger spacing

• Apply local Metropolis-Hastings algorithm where we sample on a slice-by-slice basis

• Theory shows that asymptotic convergence is unchanged

• Unfortunately larger spacing similar to less regularization

• Currently have issues with poor data models that need to be resolved
Full 3D

- In medical imaging, have multiple slice orientations (axial, sagittal, coronal)
- In seismic, vertical and horizontal shape structure expected
- With a 2.5D approach, this introduces complexity to the graph structure
Incorporating perpendicular slices

- $c_{\perp}$ is now coupled to all of the horizontal slices
- $c_{\perp}$ only gives information on a subset of each slice
- Specify edge potentials as, e.g.:

$$
\psi_{i,\perp}(\vec{c}_i, \vec{c}_\perp) = \exp(- \frac{L_y}{0} (\Gamma(x_0, y, i\Delta z) - \Gamma_{\perp}(x_0, y, i\Delta z))^2 dy)
$$
Other extensions

• Additional features can be added to the base model:
  ▪ Uncertainty on the expert segmentations
  ▪ Shape models (semi-local)
  ▪ Exclusion/inclusion regions
  ▪ Topological change (through level sets)
Conclusion

- Computationally feasible algorithm to sample from space of curves
- Approximate detailed balance
- Demonstrated utility for robustness to noise, multimodal distributions, displaying uncertainty
- Can generate arbitrary shapes with relatively complex geometry
- Conditional simulation provides a natural framework to incorporate partial user segmentations on a slice-by-slice level
Further research

• Multiple curves, known/unknown topology
• We would like $q$ to naturally sample from space of smooth curves (different perturbation structure)
• Speed always an issue for MCMC approaches
  ▪ Multiresolution perturbations
  ▪ Parameterized perturbations (efficient basis)
  ▪ Hierarchical models
• How to properly use samples?